Simulation of *Legionella* Concentration in Domestic Hot Water: Comparison of Pipe and Boiler Models

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The energy needed for the production of domestic hot water represents an important share in the total energy demand of well-insulated and airtight buildings. Domestic hot water is produced, stored and distributed above 60°C to kill *Legionella pneumophila*. This elevated temperature is not necessary for domestic hot water applications and has a negative effect on the efficiency of hot water production units.

In this paper, system component models are developed/updated with *L. pneumophila* growth equations. For that purpose different existing Modelica pipe and boiler models are investigated to select useful models that could be extended with equations for simulation of bacterial growth. In future research, HVAC designers will be able to investigate the contamination risk for *L. pneumophila* in the design phase of a hot water system, by implementing the customized pipe and boiler model in a hot water system model. Additionally it will be possible, with simulations, to optimise temperature regimes and estimate the energy saving potential without increasing contamination risk.

Keywords: domestic hot water (DHW), *Legionella pneumophila*, pipe model, boiler model, contamination risk, energy use

Introduction

Motivation

Domestic Hot Water (DHW) is an important building service in residential building typologies such as dwellings, apartments, hotels, retirement homes, as well as in sports facilities, hospitals, spas etc. (Stout and Muder, 2004).

Insulation levels and air tightness of building envelopes have been improved due to the tightening of energy performance requirements for buildings. The production of DHW, which has seen comparatively little innovation, now represents an important share of total energy demand of well-insulated and airtight buildings (Rogatty, 2003). On average, about 800kWh per occupant per year is the net energy needed for DHW production (DIN 4708-2, 1994). For a dwelling with a floor area of 170m² and 3.5 occupants (Rogatty, 2003, Delghust et al., 2015), this amounts to 15kWh/m² a year. This is the lowest (blue) bar in *Figure 1*. As can be seen in *Figure 1*, the total heating demand for buildings built before 1984 (in Germany) is 225kWh/m² a year, this means the energy needed for DHW accounts for about 6% of household energy costs, while for passive buildings this is about 50%. Additional to the rising DHW energy use in moderate or cold climates, warm climates have a limited heating demand which makes the relative share in DHW energy demand equally large or even larger (Fuentes et al., 2018).

Hot water energy demand remained unchanged over the years, while projected energy performance requirements for 2020 state to reduce the total energy demand for heating, cooling and DHW production to 1/3 of what they were in 2006.

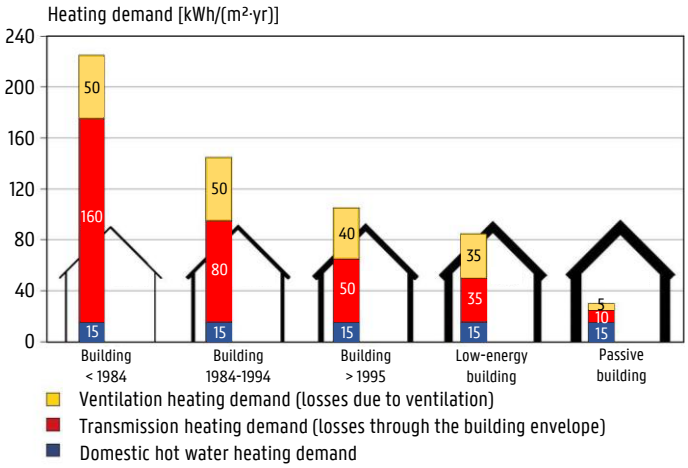

Figure 1. Comparison of heating demand (ventilation, transmission and DHW) for buildings of different age and energy efficiency level. The comparison is based on a one-family house of 150m² (A/V=0.84) with three to four occupants in Germany (adapted from Rogatty, 2003).

Problem statement

One of the main reasons for the high energy demand is that DHW is produced, stored and distributed at temperatures above 60°C to mitigate the risk of contaminating the DHW system with *L. pneumophila*. These bacteria cause, upon exposure, acute respiratory disease or severe pneumonia. At temperatures above 60°C, *L. pneumophila* growth is stopped and remaining bacteria are killed.

For most of the DHW applications, like taking a shower or washing hands, temperatures of only 30-40°C are required. This disparity (between 60°C and 40°C), doubles the temperature difference between DHW system and environment (around 20°C), which has a negative effect on distribution heat losses and on the efficiency of DHW production units such as heat pumps. With the aim of more energy-efficient buildings in mind, a straightforward strategy is to reduce temperature for hot water production whenever possible (for certain periods). For that purpose, the growth of *L. pneumophila* in systems needs to be known.

Simulating *L. pneumophila* growth in DHW systems will result in a more accurate prediction of the concentration of *L. pneumophila* in systems, which makes it possible to investigate energy saving alternatives without increasing contamination risk.

State of the art

The 60°C temperature limit has been established by investigating the growth dynamics of *L. pneumophila* bacteria in lab conditions and studying infected cases (Brundrett, 1992). No previous research has been published on modelling *L. pneumophila* on DHW system level from a combined engineering-biological point of view. Recent studies focus on the survival of *Legionella* bacteria and amoeba in biofilms (Konishi et al., 2006, Buse et al., 2014). Other research projects look at the exposure mechanics once a system is contaminated (Schoen et al., 2011, Hines et al., 2014) or focus on the influence of tubing material (Van Der Kooij et al., 2005) etc. The literature about decontamination strategies for contaminated systems is similarly scattered as that on the proliferation of *Legionella,* usually focusing on a single decontamination technique and tested in limited lab configurations or in case studies (Lehtola et al., 2005). The limitations of these studies are summarized in *Decontamination of Biological Agents from Drinking Water Infrastructure* (Szabo and Minamyer, 2014). Other papers focus on the effect of these techniques on biofilms (Mathieu et al., 2014). Reports from infection cases demonstrate that popular decontamination strategies such as applying thermal shock or chlorination often only have a temporary effect. After returning to normal use, *Legionella* growth resurfaces, probably due to flow stagnation or biofilm residue. So far, accurate information on how to incorporate dynamic temperature profiles, piping design or DHW use profiles in a risk assessment is not available, limiting design options for DHW systems and forcing the available standards to require high temperatures continuously. This is reflected for example in the REHVA

(Federation of European Heating, Ventilation and Air Conditioning Associations) handbook on *Legionella* mitigation. Although a lot is known about the growth dynamics of *Legionella*, and advances have been made in hydronic modelling allowing accurate prediction of the dynamic flow conditions (temperatures, velocities, pressures) in DHW systems (Vandenbulcke, 2013), both need to be combined in order to be able to assess the *L. pneumophila* contamination risk on system level (Van Kenhove et al., 2015).

Scope

To build a simulation model, the possibilities to model *L. pneumophila* growth in water and biofilm are investigated, and applied to pipe and boiler models.

In the first part of the paper, the theory, important to understand the simulation model, is given. This includes the explanation of *L. pneumophila* growth in water and in biofilm and ends with a figure of both growth curves, based on literature review data. Next, the theory section is translated into a model, by curve fitting of the measurements figure into temperature dependent growth equations. Mass conservation equations are given for a typical pipe and storage tank component. Further, existing Modelica pipe and storage tank components are compared and the most suitable one is chosen and adapted by adding the growth equations. The paper ends with a proof of concept in which the models are used to simulate a simple DHW system.

Methodology

A DHW system is composed of different components, for example pipes, storage tank, heat exchanger, expansion vessel, taps. In this paper, system component models are developed/updated with *L. pneumophila* growth equations. Based on water volume, the main part of the system consists of piping and in most cases a storage tank. For that purpose different existing Modelica pipe and boiler models are analysed to select useful models that could be extended with equations for simulation of bacterial growth. After selecting useful pipe and boiler models, these component models are chosen to be the first to be adapted with the implementation of the *L. pneumophila* model, as growth and exchange take mainly place in these components. The following paragraphs will show how the chosen pipe and boiler model is adapted. However, following the same logic, other Building Fluid elements for modelling thermohydraulic systems (e.g., expansion vessel, pump, heat pump) can also be easily upgraded in the same way to include *L. pneumophila* growth equations.

The benefit of modelling *L. pneumophila* growth in an existing pipe component model is the ease of compiling simulation models of different systems later on by dragging and dropping the different DHW components (which already include bacteria growth equations) into the system model.

In future research, the customized pipe and boiler model can be implemented in a hot water system model. This will make it possible to investigate the contamination risk for *L. pneumophila* in the design phase of a DHW system, while keeping an equilibrium between healthy buildings and energy efficiency, without compromising on health. Additionally it will be possible, with simulations, to estimate the energy saving potential without increasing contamination risk.

The growth curves in the simulation components are validated in this paper based on literature data and the use of these components in different system simulation models will be validated in future research based on test rig and case study measurements.

Theory

In literature, there are no previous attempts to model the dependencies between *L. pneumophila* growth and energy efficiency, probably because the topic requires a multidisciplinary approach. This is the first time, to the authors' knowledge, a dedicated simulation model is made. The biological growth model is made up of a number of sub-equations: growth and transport of *L. pneumophila* in water, *L. pneumophila* growth in biofilm and bacteria transport between biofilm and water.

To model the proliferation of *L. pneumophila* in water, it is modelled as a trace substance in different DHW components, for example a pipe and a boiler. Based on a literature review, the main parameters that have an impact on the multiplication of *L. pneumophila* bacteria are selected and added to the model as equations. This includes the equations of dependency between *L. pneumophila* growth, water temperature and flow conditions.

Legionella pneumophila growth in water

Multiplication of *L. pneumophila* is dependent on water temperature, volume flow rate, flow frequency, followed by nutrient availability (Völker et al., 2015). At temperatures below 20°C, the bacteria become dormant but remain viable for months. The bacteria grow best at temperatures between 20°C and 45°C with an optimum around 35°C-41°C. Beyond 45°C, pasteurization starts and higher temperatures will eventually kill the organisms (Brundrett, 1992). This can be seen on *Figure 2* and *Figure 3*. *Figure 2* is

based on data from Yee and Wadowsky (1982) from experiments on unsterilized tap water and *Figure 3* is based on data from laboratory experiments (Dennis et al., 1984, Stout et al., 1986, Schulze-Röbbecke et al., 1987, Sanden et al., 1989), and is consistent with field data (Groothuis et al., 1985). On the x-axes, the water temperature in degrees Celsius can be seen and on the y-axes, in *Figure 2,* the time to double the number of *L. pneumophila* (mean generation time) and, in *Figure 3,* the time to reach 90% reduction in cells (decimal reduction time). *Figure 2* shows that the time to double the number of *L. pneumophila* cells in water is less than half a day at 41°C and in *Figure 3* it can be noted that at 70°C, 90% of *L. pneumophila* in water gets killed in less than a minute. The growth/death rate at any temperature is proportional to the number of living cells present (Reddish, 1957, Sykes, 1965, Allwood and Russell, 1970) (*Equation 1*).

Growth/death rate: $$\frac{dC(t)}{dt} = A(T) \cdot C(t) - B(T) \cdot C(t) \quad (1)$$

Number of cells: $$C(t) = C_0 \cdot e^{(A(T)-B(T)) \cdot t}$$

With:

- *A(T)* [-] Growth function depending on water temperature, the species of the organism and the chemical nature of the water
- *B(T)* [-] Death function depending on water temperature, the species of the organism and the chemical nature of the water
- C_0 [cfu/m³] Start concentration of *L. pneumophila* in water entering the system
- *C(t)* [cfu/m³] Concentration of *L. pneumophila* in water at time *t*
- *dC(t)/dt* [cfu/s] Change in concentration of *L. pneumophila* over time
- *t* [s] Time

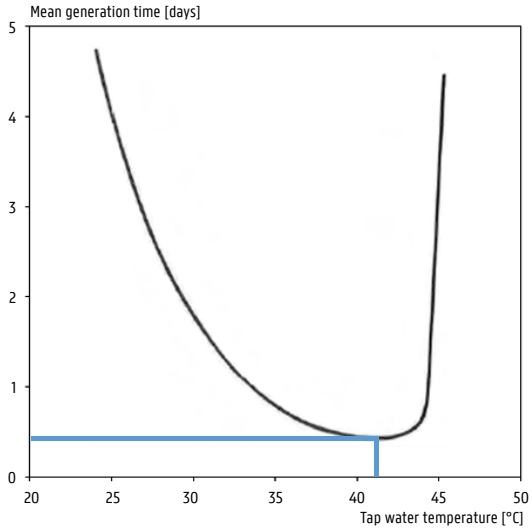

Figure 2. An estimation of mean generation time (time to double the number of cells) of *L. pneumophila* in tap water (data from Yee and Wadowsky, 1982, adapted from Brundrett, 1992).

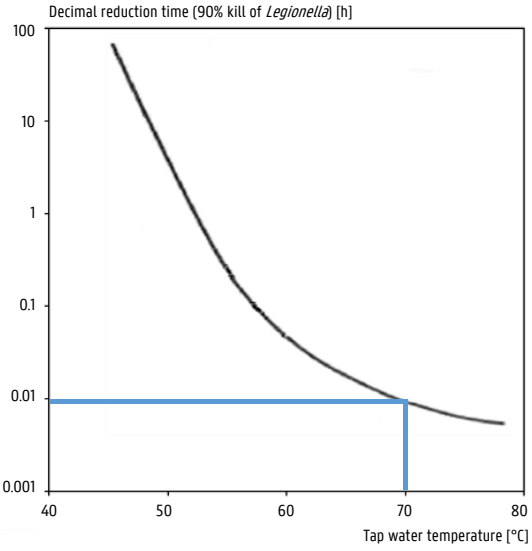

Figure 3. The change in decimal reduction time (90% reduction of *L. pneumophila*) with temperature (data from Dennis et al., 1984, data from Stout et al., 1986, adapted from Brundrett, 1992).

Legionella pneumophila growth in biofilm

An uncritical natural concentration of *L. pneumophila* enters the building, if the conditions in these man-made environments are optimal for bacterial growth, it can reach dangerous concentrations. If *L. pneumophila* would appear only in water, it would

be flushed out of the system during water use and would not have time to grow. However, DHW system component models do not only contain water, but also biofilm (*Figure 4).*

What is a biofilm?

A biofilm is a slimy layer of microorganisms present inside for example water pipes. This layer can be as thin as a single cell attached to the surface (<5µm) and as thick as 1 000µm (Murga et al., 1995).

Wherever there is water, biofilm growth can occur, for example in storage tanks, humidifiers and cooling towers. Biofilms can grow easily in DHW pipes since they provide a moist and warm environment for the biofilm to thrive. Modelling of the biofilm is important because 95% of *L. pneumophila* are biofilm-associated (Flemming, 2002).

Figure 4. *L. pneumophila* in water (left graph with blue contour) and *L. pneumophila* attached in biofilm (right graph with brown contour). The colors of these figures are used throughout the paper to indicate in a quick visual way if a curve is obtained for water or biofilm.

The biofilm structure is composed of a consortium of microbial cells that are attached to the surface (substratum) and associated together in an extracellular anionic polymer matrix (Donlan, 2002). The matrix is extremely hydrated (97% water) (Farhat et al., 2012). Micro colonies of bacterial cells encased in the extracellular anionic polymer matrix are separated from each other by interstitial water channels, allowing transport of

nutrients, oxygen, genes and even antimicrobial agents (Prakash et al., 2003). Because of their dynamic character, biofilm communities can continuously change over time and space, providing better survival and growth of the associated microorganisms (Declerck, 2010). *L. pneumophila* bacteria attach to the biofilm because it consists of microorganisms that allow cells to adhere to the pipe surface. Generally, there are three distinct phases in the biofilm life cycle of *L. pneumophila* (Donlan, 2002): bacterial attachment to a substratum, biofilm maturation and detachment from the biofilm, which means dispersal in the bulk environment.

Protective function of the biofilm

The biofilm forms a protective layer for *L. pneumophila* that allows them to grow and multiply within the biofilm. First, several authors have reported that *L. pneumophila* bacteria living in a biofilm are more resistant to environmental stress and water decontamination treatments (Fields et al., 1984, Sanderson et al., 1997, Sutherland, 2001, Russell, 2003, Borella et al., 2004, Van Der Kooij et al., 2005, Cervero-Aragó, 2015). This means for example a better resistance to higher temperatures. Secondly, *L. pneumophila* is able to infect and replicate inside protozoans, which can survive as an intracellular parasite of free-living amoebae (Rowbotham, 1980, Altschul et al., 1990, Kilvington et al., 1990, Thomas et al., 2004, Wéry et al., 2008, Farhat et al., 2012). Free-living amoebae are eukaryotic microorganisms that are commonly found in drinking water systems, and more specifically in biofilms. This association established between *L. pneumophila* and amoebae in biofilm in DHW systems indicates an increased health risk because amoebae provide an ideal growth environment making *L. pneumophila* bacteria more resistant to environmental stress and water decontamination treatment.

Effect of temperature on Legionella pneumophila in biofilm

Cervero-Aragó et al. (2015) tested the effect of temperature on a *L. pneumophila* strain and two amoebae strains under controlled laboratory conditions. To determine the influence of the relationship between *L. pneumophila* and amoebae *Acanthamoeba species* and *Acanthamoeba Castellani* on the treatment effectiveness, inactivation models of the bacteria-associated amoeba were constructed and compared to the models obtained for *L. pneumophila* living freely in water.

The thermal treatment was tested at four experimental temperatures: 50°C, 55°C, 60°C and 70°C, for various exposure times and applied to *L. pneumophila* under controlled laboratory conditions. *Table 1* lists the results and the R^2 values which show the robustness of the regression models.

Table 1. Calculated time for a 4 log reduction of *L. pneumophila serogroup 1* environmentally associated with *Acanthamoeba Castellani CCAP 1534/2* and *Acanthamoeba species 155* after the exposure to different temperatures (adapted from Cervero-Aragó et al., 2015).

Calculated time to reduce 4 logs [minutes]				
Effect of temperature on free *Legionella*	**50°C (R^2)**	**55°C (R^2)**	**60°C (R^2)**	**70°C (R^2)**
L. pneumophila sg. 1 env (Axenic)	46 (0.84)	8 (0.98)	4 (0.86)	0.61 (0.82)
Effect of temperature on amoebae-associated *Legionella*	**50°C (R^2)**	**55°C (R^2)**	**60°C (R^2)**	**70°C (R^2)**
L. pneumophila sg. 1 env - *A. Castellani* CCAP 1534/2	825 (0.56)	45 (0.84)	5 (0.99)	0.45 (0.82)
L. pneumophila sg. 1 env - *Acanthamoeba* sp. 155	664 (0.95)	51 (0.95)	5 (0.73)	0.50 (0.92)

The results in the upper section of *Table 1* are comparable with the results of *Figure 5* (blue curve). We are especially interested in the effect of temperature on *L. pneumophila* inside amoebae, this can be seen in the lower section in *Table 1*. The effectiveness of the thermal treatment on the amoebae-associated *L. pneumophila* compared to the free living *L. pneumophila* was reduced. At 50°C, the *L. pneumophila* resistance (measured in time) was increased 14 to 18 times, and at 55°C it was increased 5 to 6 times. Thus, it seems that *Acanthamoeba* and *A. Castellani* strains are protecting *L. pneumophila* at temperatures below 60°C, but at higher temperatures, its protection

decreases enormously (Cervero-Aragó et al., 2015).

Figure 5 shows the temperature dependent growth function of *L. pneumophila* in water (blue) and in biofilm (brown). The biofilm curve is an estimation established based on the review results of available literature (Storey et al., 2004, Cervero-Aragó et al., 2015). The study of Cervero-Aragó et al. (2015) shows the time required to reach a 4 log reduction for the *Axenic L. pneumophila sg 1*, when *L. pneumophila* was associated with either *Acanthamoeba* or *A. Castellani* (in biofilm). The most negative data (slowest death rate) of the *Legionella*-amoebae association is plotted into the brown curve. There is no data available for the growth of *L. pneumophila* in biofilm between 20 and 35°C. However, it is known from literature that the multiplication rate of *L. pneumophila*, between 20°C and 30°C, is higher if it is present in biofilm compared to water (Storey et al., 2004), but we cannot yet quantify it. Based on future biological research this part of the growth curve can be replaced at a later stage.

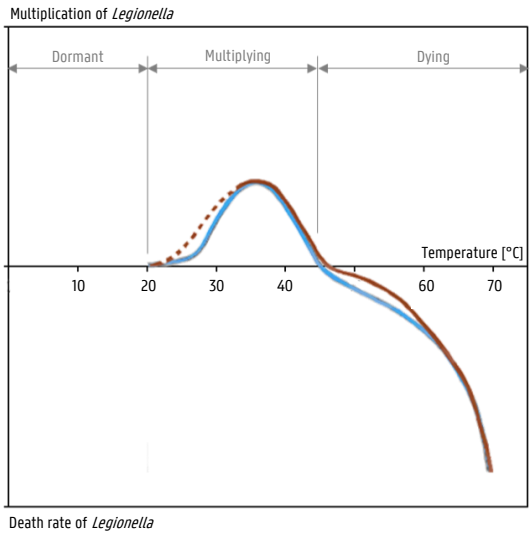

Figure 5. Growth function of *L. pneumophila* in water (blue) (Brundrett, 1992) and in biofilm (brown) (assumption derived from Storey et al., 2004, Cervero-Aragó et al., 2015).

Simulation and experiment

Modelling of Legionella pneumophila in DHW components

Figure 6 shows the modelling approach for *L. pneumophila* concentrations in pipe models and *Figure 7* in boiler models. The blue colour represents water, the brown colour represents the biofilm.

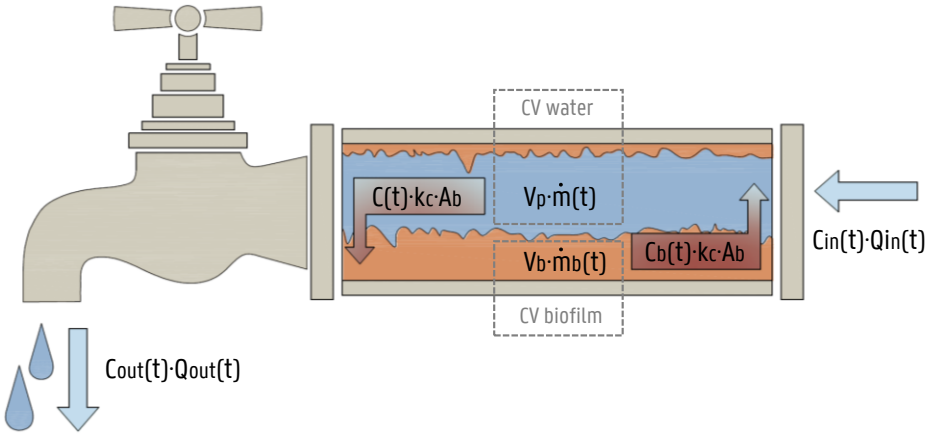

Figure 6. Concentration of *L. pneumophila* in water (blue) and biofilm (brown) of DHW pipe, shown as dual Control Volume (CV) scheme.

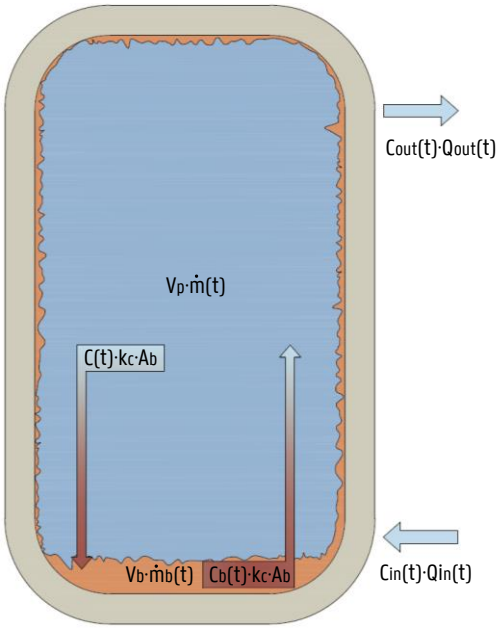

Figure 7. Concentration of *L. pneumophila* in water (blue) and biofilm (brown) of DHW boiler, shown as dual CV scheme.

To model *L. pneumophila* growth in **water** in a pipe or boiler, equations need to be added to the hydraulic model. Following mass conservation equations, that predict *L. pneumophila* growth in water, need to be coupled to an existing pipe or boiler component (*Equation 2, Equation 3, Equation 4*).

$$V_p \cdot \frac{dC(t)}{dt} = C_{in}(t) \cdot \frac{Q_{in}(t)}{\rho} - C_{out}(t) \cdot \frac{Q_{out}(t)}{\rho} + growth\ in\ water + mass\ transfer\ between\ water\ and\ biofilm$$

$$\Leftrightarrow V_p \cdot \frac{dC(t)}{dt} = C_{in}(t) \cdot A_{in} \cdot \vec{v}_{in}(t) - C_{out}(t) \cdot A_{out} \cdot \vec{v}_{out}(t) + V_p \cdot \dot{m}(t) + k_c . A_b . (C_b(t) - C(t)) \quad (2)$$

$$Q_{in}(t) = Q_{out}(t) \quad (3)$$

$$\dot{m}(t) = C_{previous} \cdot \frac{ln(2)}{y} \cdot e^{\frac{ln(2)}{y} dt} \quad (4)$$

With:

- A_b [m²] Surface between water and biofilm
- $C(t)$ [cfu/m³] Concentration of *L. pneumophila* in water at time *t*
- $C_{in}(t)$ [cfu/m³] Concentration of *L. pneumophila* in water entering system
- $C_{out}(t)$ [cfu/m³] Concentration of *L. pneumophila* in water leaving system
- $C_b(t)$ [cfu/m³] Concentration of *L. pneumophila* in biofilm at time *t*
- $C_{previous}$ [cfu/m³] Concentration of *L. pneumophila* in water on previous timestep. $C_{previous} = C_{b,0}$ on first timestep
- $dC(t)/dt$ [cfu/m³·s] Changing concentration of *L. pneumophila* over time
- k_c [m/s] Mass transfer coefficient to calculate the mass transfer of *L. pneumophila* between water and biofilm
- $\dot{m}(t)$ [cfu/s] Change in concentration of *L. pneumophila* due to growth or death
- $Q_{in}(t)$ [kg/s] Mass flow rate of water (containing *L. pneumophila)* entering system
- $Q_{out}(t)$ [kg/s] Mass flow rate of water (containing *L. pneumophila)* leaving system
- T [K] Absolute temperature
- t [s] Time
- Δt [s] Timestep
- V_p [m³] Volume of water in pipe or boiler
- $\vec{v}_t$ [m/s] Mass-average velocity for multicomponent mixture
- y [s] Multiplication time of *L. pneumophila* in water dependent on temperature
- ρ [kg/m³] Mass density of mixture

To model *L. pneumophila* growth in **biofilm** in a pipe or boiler, equations need to be added to the hydraulic model in a similar way as for growth in water. Following mass

conservation equations, that predict *L. pneumophila* growth in biofilm, need to be coupled to an existing pipe or boiler component (*Equation 5*, *Equation 6*, *Equation 7*).

$$V_b \cdot \frac{dC_b(t)}{dt} = C_{b,in}(t) \cdot \frac{Q_{b,in}(t)}{\rho} - C_{b,out}(t) \cdot \frac{Q_{b,out}(t)}{\rho} + growth\ in\ biofilm + mass\ transfer\ between\ biofilm\ and\ water$$

$$\Leftrightarrow V_b \cdot \frac{dC_b(t)}{dt} = C_{b,in}(t) \cdot A_{b,in} \cdot \vec{v}_{b,in}(t) - C_{b,out}(t) \cdot A_{b,out} \cdot \vec{v}_{b,out}(t) + V_b \cdot \dot{m}_b(t) + k_c . A_b(C(t) - C_b(t)) \quad (5)$$

$$Q_{b,in}(t) = Q_{b,out}(t) = 0 \quad (6)$$

$$\dot{m}_b(t) = C_{b,previous} \cdot \frac{ln(2)}{y_b} \cdot e^{\frac{ln(2)}{y_b} dt} \quad (7)$$

With:

- A_b [m²] Surface between biofilm and water
- $C_b(t)$ [cfu/m³] Concentration of *L. pneumophila* in biofilm at time *t*
- $C_{in}(t)$ [cfu/m³] Concentration of *L. pneumophila* in biofilm entering biofilm segment
- $C_{out}(t)$ [cfu/m³] Concentration of *L. pneumophila* in biofilm leaving biofilm segment
- $C_{b,previous}$ [cfu/m³] Concentration of *L. pneumophila* in biofilm on previous timestep. $C_{b,previous} = C_{b,0}$ on first timestep
- $dC_b(t)/dt$ [cfu/m³·s] Changing concentration of *L. pneumophila* in biofilm over time
- $\dot{m}_b(t)$ [cfu/m³·s] Change in concentration of *L. pneumophila* in biofilm due to growth or death
- $Q_{b,in}(t)$ [kg/s] Mass flow rate of water (containing *L. pneumophila)* entering biofilm
- $Q_{b,out}(t)$ [kg/s] Mass flow rate of water (containing *L. pneumophila)* leaving biofilm
- V_b [m³] Volume of biofilm in pipe or boiler
- $\overrightarrow{v_b}(t)$ [m/s] Mass-average velocity for multicomponent mixture
- y_b [s] Multiplication time of *L. pneumophila* in biofilm dependent on temperature

As can be seen in *Equation 6*, mass flow between different biofilm segments is not taken into account.

Determining multiplication time (y and y_b)

The rate of increase of *L. pneumophila* is temperature dependent. Because it is necessary to know the growth rate at every timestep, a function is created in Modelica which returns the growth rate *y* and y_b. Growth coefficient *y* is a time constant [s]

to predict growth or death of *L. pneumophila* in water. *y* in *Equation 4* is dependent on water temperature *T* in the pipe or boiler component. Equations of *y* are made for *L. pneumophila* in water, based on a function that fits a polynomial through the defined points in modelica, i.e., a vector containing temperature points and a vector containing the corresponding concentration of *L. pneumophila*. The points are coming from the curve presented in literature in *Figure 2* and *Figure 3*, used with an interval of 1K as shown in *Annex 2 Table 10*. Growth coefficient y_b is a function to predict growth or death of *L. pneumophila* in biofilm. y_b in *Equation 7* is dependent on water temperature *T* in the pipe or boiler component. Growth coefficients are added for growth of *L. pneumophila* in biofilm based on the results of Cervero-Aragó (2015). *Annex 1 Equation 10* shows the equations of y_b for *L. pneumophila* in biofilm, based on piece-wise fitting of the curve in *Figure 2* (growth) and measurement points presented in literature and *Table 1* (death).

A third degree piece-wise polynomial fitting technique (cubic hermite spline) was chosen in Modelica for constructing a smooth curve through the defined points. In total four different functions were developed: a separate function for the *L. pneumophila* growth and death, each of them for *L. pneumophila* in water and for *L. pneumophila* in biofilm. Several approaches have been tested, the current approach seems to have the fewest drawbacks. The flexible use of the models is the reason to choose the current approach. The advantage of using this approach, is that the user can easily adapt each curve based on his own measurement points or new findings, or for another type of bacteria.

Parameter V_b (volume of biofilm)

The parameter V_b in *Equation 5* needs some more explanation. One of the difficulties arising when taking the biofilm roughness into account is that a water pipe may be

smooth on installation and then progressively acquire a layer of calcium compounds which make the surface rough and facilitate the growth of biofilm. The predicted human contamination risk needs to be as low as possible, that is why the most negative situation is modelled (biggest system contamination risk). For this purpose, a fully developed biofilm is taken into account in the simulation models. The volume of biofilm is a percentage of the pipe volume. This can be updated later on in function of the pipe diameter. Although this simplification is made, it is important that the chosen pipe and boiler models take material roughness into account, in this way the current simplification can be updated by making biofilm thickness function of the pipes roughness/pipe material.

Parameter k_c (bacterial mass transfer coefficient)

Another parameter in the biologic model is the mass transfer coefficient k_c. The bacterial exchange between biofilm and the main water volume can be expressed with the rate equation for convective mass transfer. This equation, generalized in a manner analogous to Newton's law of cooling, is (Welty et al., 2008):

$$N_A = k_c \cdot \Delta c_A$$

With:

- N_A [mol/m²·s] Molar-mass flux of the species A, measured relative to fixed spatial coordinates
- Δc_A [mol/m³] Concentration difference between boundary surface concentration and average concentration of diffusing species in moving fluid stream
- k_c [m/s] Convective mass-transfer coefficient

The method used to determine the mass transfer of bacteria between biofilm and water is based on the boundary layer theory (Prandtl, 1904). The boundary layer is the thin region of flow adjacent to the biofilm surface, where the flow velocity is dependent of friction between the biofilm surface and the water (momentum boundary layer) and

where energy transfer (thermal boundary layer) and mass transfer (concentration boundary layer) occur. The Reynolds analogy states that the mechanisms for transfer of momentum and energy in the momentum and thermal boundary layer are identical if the Prandtl number *Pr* equals 1 and that the momentum and thermal boundary layer thickness are more or less equal. The Prandtl number for water is 4-7. In Welty et al. (2008), this postulation is extended with mass transfer in case the Schmidt number *Sc* is unity. For water however the Schmidt number is around 540. This Schmidt number plays a role in convective mass transfer in the same way as the Prandtl number in convective heat transfer. It can be expressed as the ratio of the molecular diffusivity of momentum to the molecular diffusivity of mass. Using these analogies, a relation between the different transport phenomena is expressed.

Since the Reynolds analogy is only valid for gases (*Pr* = 1 and *Sc* = 1), Chilton and Colburn suggested an equation which makes it possible to extend the Reynolds analogy to liquids by eliminating the restriction of unity of Prandtl and Schmidt numbers (Colburn et al. 1933, Chilton et al., 1934). This analogy is valid for gases and liquids within the range $0.6 \leq Sc < 2\,500$. The convective mass transfer coefficient k_c can be obtained from the skin friction coefficient C_f of the boundary layer and the Schmidt number *Sc*:

$$\frac{k_c}{v_\infty} = \frac{C_f}{2} \cdot \frac{1}{Sc^{2/3}}$$

With v_∞ [m/s] the velocity in the centre of the pipe.

For a laminar boundary layer, the skin friction coefficient was determined by Blasius (1908).

$$C_f = \frac{1.328}{\sqrt{Re}}$$

For a turbulent boundary layer, different approximate solutions exist to calculate the skin friction coefficient. In this work the Prandtl-Schlichting equation (Schlichting et al., 1979), which uses a logarithmic velocity profile, is used. It is valid if Re < 10^9:

$$C_f = \frac{0.455}{(\log Re)^{2.58}}$$

Parameter K (carrying capacity)

At certain critical temperatures, there is an unlimited increase of *L. pneumophila* concentration in *Equation 1* where in reality after a while a stabilization in concentration will be noticed. This occurs because the system can only hold as many *L. pneumophila* bacteria as nutrients and oxygen can support. To take nutrients into account, parameter *K*, the carrying capacity, is added to the mass conservation equation (Verhulst-Pearl logistic equation) (Panikov, 1995). It can be modelled with the Verhulst-Pearl logistic equation, that is sigmoidal (S-shaped) and reaches an upper limit at *K*. *K* is the maximum concentration of *L. pneumophila* that oxygen and nutrients can support. *L. pneumophila* concentrations above *K* decline exponentially until they reach the stable equilibrium *K* (Panikov, 1995) (*Equation 8*). The definition of *A(T)*, *B(T)* (Growth/death function depending on water temperature, the species of the organism and the chemical nature of the water) can be seen in *Equation 1*.

$$\frac{dC(t)}{dt} = A(T) \cdot C(t) \cdot (1 - \frac{C(t)}{K}) \text{ (growth)}$$
$$\frac{dC(t)}{dt} = B(T) \cdot C(t) \cdot (1 - \frac{C(t)}{K}) \text{ (death)} \quad (8)$$

To take *K* into account, *Equation 4* and *Equation 7* become *Equation 4'* and *Equation 7'* respectively.

$$\frac{\dot{m}(t)}{\dot{m}(t)-K} = \frac{C_{previous}}{C_{previous}-K} \cdot e^{\frac{ln(2)}{y} \cdot dt} \quad (4')$$

$$\frac{\dot{m}_b(t)}{\dot{m}_b(t)-K} = \frac{C_{b,previous}}{C_{b,previous}-K} \cdot e^{\frac{ln(2)}{y_b} \cdot dt} \quad (7')$$

To find the most suitable pipe and boiler component for this simulation purpose, a

comparative study is performed within the Modelica environment. First of all, a suitable simulation environment and libraries are chosen. Subsequently, an adequate pipe and boiler component is chosen.

Modelica simulation environment

Within the scope of this work, the following criteria were considered in first selecting the simulation tool and secondly the components. These criteria are requirements for the *L. pneumophila* growth model.

This is the first work to the authors' knowledge that models *L. pneumophila* in DHW systems. This means assumptions need to be made for some biological parameters. As more biological research on these parameters is needed, this simulation model can be considered as a framework for other researchers to overwrite the assumptions. Therefore the modelling language should be open source and it should be possible to adapt the code easily.

The goal is to have one tool that is flexible and that can be used for multiple scales, from a whole building's DHW system to *L. pneumophila* growth in a small water/biofilm segment, and in multiple contexts, from design to decontamination. Having a large number of different tools work together in such conditions is generally perceived to be much less stable. Additionally, it requires the users to be acquainted with all different simulation packages and is less flexible towards extensions of the model to other situations.

Other boundary conditions are:

- The model will be used in simulations of the DHW system of a building as a whole or as a part of it. It is not necessary to model the building's envelope and other installation.

- The modelling tool has to estimate short-term *L. pneumophila* growth (water usage is second based), as well as long-term growth (effect of number of heat shocks). In other words, it should be able to do a non-steady calculation of the building's DHW system for one day to one month (timestep of 0.1-1 second for numerical stability).
- The simulation tool has to be fast, the calculation of *L. pneumophila* growth combined with one retrofitting option for a case study apartment building (of 200 apartments) with collective DHW system should be performed in maximum 24 hours. This is necessary to use the simulation model in decontamination consultancy, where time is crucial.
- It should be possible to perform the calculations on a 'standard' laptop (8GB RAM - CPU 2 cores - 2.67 GHz). This is necessary to guarantee a broad use of the simulation model in design and decontamination consultancy. For complex systems, an exception can be made.

To meet these requirements, the simulation model is written in the Modelica language and compiled in the Dymola environment (Modelica, 2016). This equation based programming language is non-proprietary and object oriented. It also contains different existing libraries, hydraulic as well as biologic, making it appropriate for the development of multi-scale (thermohydraulic and biologic) models such as are required here. This work adds to the capabilities of the Modelica models by providing a biological growth library that was not available before. Modelica's open source and modular structure will allow users to use this library to model similar biological growth problems in all kinds of applications.

Extensive libraries for simulation of buildings and their services have been developed in IEA EBC Annex 60 (Annex 60, 2012). The Annex 60 integrated core

libraries are compatible with other Modelica building energy simulation libraries. For this study existing pipe and boiler models of the standard Modelica (3.2.1) library and of two libraries developed in Annex 60, namely OpenIDEAS (0.3.0) library and integrated Buildings (3.0.0) library, are compared because all three libraries contain building as well as system component models for energy performance simulation (Wetter et al., 2014, Jorissen et al., 2018).

Comparison of pipe and boiler models in Modelica

There are a number of parameters necessary for modelling bacteria growth. The parameters are divided into three categories, namely the three conservation equations: mass conservation (differential continuity equation, *Annex 3 Equation 31*), momentum conservation (Newton's 2nd law of motion, Navier-Stokes equation, *Annex 3 Equation 32*) and energy conservation equation (*Annex 3 Equation 33*). It is studied how the existing models deal with these conservation equations. The conversion from the general form of the conservation equation to the equations with parameters used in the Modelica simulation environment can be found in *Annex 5*. When referring to different parameters below, the parameter names defined in Modelica are used.

To select the pipe and boiler models, following assumptions were made. First of all, the pipe model has to be a 1D flow model, this means that the velocity in the x-direction dominates the flow, meaning the velocity in y- and z-direction is negligible, allowing the equations to be transformed to 1D. This means that CFD-models are not considered. The second assumption made is that water is incompressible.

The mass conservation parameter 'trace substances' indicates if the existing pipe component contains certain flow equations that make it possible to add substances to water. This is the most important parameter related to the addition of *L. pneumophila*, this is the parameter the growth equations need to be coupled with.

Momentum conservation parameter ‘gravity’ defines if the pipe can be used in all directions (vertical/horizontal). A pipe model without inclusion of gravity can only be used horizontally, except if the gravity equation is overruled by the pressure drop. ‘Pressure drop’ inclusion is important because it influences the fluid flow, which in return influences mass transfer between biofilm and water. The momentum conservation parameter ‘state of the flow (laminar/turbulent)’ is a meaningful parameter for the purpose of this research because *L. pneumophila* growth is flow dependent, as this influences the amount of bacteria attaching to and detaching from the biofilm into the bulk liquid phase. Momentum conservation parameters like ‘friction’ and ‘material roughness’ are important parameters in a pipe component because these parameters influence the amount of biofilm formation.

Energy conservation parameters, for example the possibility to add a ‘heat source’ and ‘insulation’, are meaningful parameters to take into account. They assure that the pipe and boiler can be used in as many system configurations as possible. ‘nNodes’ means that the pipe can be divided into a predefined number of volume segments. ‘Heat exchange’ is the exchange of heat with the environment. This is an important part of the model to match real conditions as it influences water temperature, which in its turn affects the growth or death of *L. pneumophila* bacteria.

It is not necessary to add other new parameters for bacteria growth to the momentum and energy conservation equations, such as the parameter for *L. pneumophila* growth added to the model in the mass conservation equation. However, it is necessary to compare the inclusion of these parameters in the different models because they are of interest for the growth equations and mass transfer between water and biofilm (*Equation 2* and *Equation 5*). For example, the volume of the biofilm

changes according to the material roughness. So material roughness should be accessible as a parameter in the chosen pipe and boiler model.

Comparison of pipe models

Existing pipe models were compared based on the above parameters necessary for modelling bacteria growth and that may or may not have been taken into account in the conservation equations in the existing component models.

By comparing these parameters, the existing pipe models that can be extended with equations for simulation of bacterial growth in DHW are selected. *Table 2* gives an overview of all selected existing pipe models (ranked according to the library to which they belong) and the presence of the necessary parameters. If the parameter is indicated by '1' (green) it has been taken into account, if it is indicated by '0' (red), the parameter is not part of the existing model.

Out of the comparison of the different pipe models in *Table 2*, the authors chose to adapt the 'Pipe' model from the Buildings (3.0.0) library because the most important parameters are taken into account in the model. Gravity equations are missing from this Pipe component, these can be added in a similar way as in the Dynamic pipe model. However, it needs to be mentioned that the influence of adding this parameter is small because for DHW applications, flow is dominated by pressure by using a pump (parameter: pressure drop). Three other pipe models are suitable for the authors' applications: Dynamic pipe, Insulated pipe and Pipe insulated. The reason not to retain them is described in *Annex 4*.

Table 2. Comparison of DHW pipe component models based on parameters for bacteria growth modelling.

Data			Mass balance	Momentum balance					Energy balance			
Name	**Library**	**Description**	**Trace substances**	**Gravity**	**Pressure drop**	**Laminar/ turbulent flow**	**Friction**	**Material roughness**	**Heat source**	**Heat exchange**	**Insulation**	**nNodes**
Dynamic pipe 	Modelica 3.2.1	Dynamic pipe model with storage of mass and energy	1	1	1	1	1	1	0	1	0	1
Static pipe 	Modelica 3.2.1	Basic pipe flow model without storage of mass or energy	0	1	1	0	1	1	0	0	0	0
Heated pipe 	Modelica 3.2.1	Pipe with heat exchange	0	1	1	1	1	0	1	1	0	0
Isolated pipe	Modelica 3.2.1	Pipe without heat exchange	0	1	1	0 (only laminar)	1	0	0	0	0	0
Short pipe 	Modelica 3.2.1	Simple pressure loss in pipe	0	0	1	0	1	0	0	0	0	0
Embedded pipe 	OpenIDEAS 0.3.0	Embedded pipe model based on prEN 15377 and (Koschenz, 2000)	1	0	1	1	1	1	0	1	1	0
Insulated pipe 	OpenIDEAS 0.3.0	Insulated pipe characterized by UA	1	0	1	1	1	0	0	1	1	0
Pipe 	OpenIDEAS 0.3.0	Pipe without heat exchange or pressure drop	1	0	0	0	0	0	0	0	0	0
Pipe heatport 	OpenIDEAS 0.3.0	Pipe with HeatPort	1	0	1	1	1	0	0	1	0	0
Pipe insulated	OpenIDEAS 0.3.0	Pipe with insulation, characterized by UA	1	0	1	1	1	0	0	1	1	0
Lossless pipe 	OpenIDEAS/ Buildings 3.0.0	Pipe with no flow friction and no heat transfer	0	0	0	0	0	0	0	0	0	0
Pipe 	Buildings 3.0.0	Pipe with finite volume discretization along flow path	1	0	1	1	1	1	0	1 (multiple heat ports)	1	1

Comparison of boiler models

Next to pipe models, existing boiler models were compared based on the parameters for bacteria growth modelling. In case of boilers an additional parameter which is important for modelling the growth and displacement of *L. pneumophila* is 'stratification of the boiler'.

Table 3 gives an overview of all selected existing boiler models, the library to which they belong and the presence of the necessary parameters. If the parameter is indicated by '1' (green) it is taken into account, if it is indicated by '0' (red), the parameter is not part of the existing model.

Out of the comparison of the different boiler models in *Table 3*, the 'StratifiedEnhancedInternalHex' boiler model, of the Buildings library 5.0.1, is chosen as most suitable for the authors' applications because it meets most of the requirements and is a stratifying boiler. As well as the Pipe model, it contains a Mixing Volume component which will be used to implement the growth equations (see *Implementation*). Reasons why not to retain certain other models are mentioned in *Annex 4*.

Other DHW components, like heat exchangers, expansion vessels, water softeners etc. are not, but the modelling approach is similar.

Table 3. Comparison of DHW boiler component models based on parameters for bacteria growth modelling.

Data			Mass balance	Momentum balance					Energy balance				Strati-fication
Name	**Library**	**Description**	**Trace substances**	**Gravity**	**Pressure drop**	**Laminar/ turbulent flow**	**Friction**	**Material roughness**	**Heat source**	**Heat exchange**	**Insulation**	**nNodes**	
Boiler 	OpenIDEAS 0.3.0	Modulating boiler with losses to environment, based on performance tables	1	0	1	1	0	0	1	1	0	0	0
Boiler Polynomial 	Buildings 3.0.0	Boiler with efficiency curve described by a polynomial of the temperature	1	0	1	1	0	0	1	1	1	0	0
OpenTank 	Modelica 3.2.1	Simple tank with inlet/outlet ports	1	0	1	1	0	0	0	1	0	0	0
Storage Tank 	OpenIDEAS 0.3.0	1D multinode stratified storage tank	0	0	0	0	0	0	0	1	1	1	1
Storage Tank_One IntHX 	OpenIDEAS 0.3.0	1D multinode stratified storage tank with one internal heat exchanger (HX)	0	0	0	0	0	0	1	1	1	1	1
Stratified Enhanced Internal Hex 	Buildings 3.0.0	A model of a water storage tank with a secondary loop and internal heat exchanger	1	0	1	1	1	0	1	1	1	1	1

Implementation of *Legionella pneumophila* equations

Medium with Legionella pneumophila and nutrients

Modelica has a modular approach, meaning that a whole DHW system is modelled by connecting several components. A Medium flows through the different components. The Buildings Fluid components make use of a Mixing Volume, equivalent to a Control Volume (CV) with a replaceable Medium. For this application a new Medium is defined starting from the Buildings.Media.Water to which two trace substances are added, namely *L. pneumophila* and nutrients. By doing so, two additional mass conservation equations are added. This updated Medium has to be used in every component of the simulated hydraulic system.

Modelica library with L. pneumophila growth and nutrients models

However, the addition of two trace substances (*L. pneumophila* and nutrients) to the Medium water are not sufficient to calculate the *L. pneumophila* concentration in a hydraulic system as the growth and mass transfer equations (*Equation 2*, *Equation 5*) are not included.

Therefore, a new library is developed consisting of new functions, models and extended components to predict *L. pneumophila* growth. Equations have to be added to include the *L. pneumophila* growth in water/biofilm and the mass exchange between water and biofilm. To include the necessary equations, two new models are developed: one including equations for the concentration of *L. pneumophila* (upper icon highlighted in yellow in *Figure 8* and *Figure 9*) and one including equations for the concentration of nutrients (lower icon highlighted in yellow in *Figure 8* and *Figure 9*). By implementing the *L. pneumophila* and nutrients model as a partial model and by extending the original

models of the component models, flexible use of the model is allowed. Moreover, it is implemented in such a way, that computation of *L. pneumophila* could be conditionally disabled. Additionally, in case the user wants to calculate more or other concentrations, equations could be added in the same way.

Pipe model implementation

Figure 8 shows the modification of the customized Pipe model from the Buildings (3.0.0) library. *Figure 8A* demonstrates the visual representation of the customized pipe element (icon view). The brown rectangles visually represent the addition of biofilm and the black circles the exchange of bacteria between biofilm and water. *Figure 8B*, showing the diagram view of the pipe, illustrates how the original Pipe model is adapted to include the thermohydraulic and biologic equations. As can be noticed, the new *L. pneumophila* and nutrients models described above are added to the pipe model of the Buildings Fluid library. These models contain *Equations 2-8*. For someone unfamiliar with the Modelica modeling software, an explanation of each symbol used in *Figure 8B* is given in *Annex 5 Table 11*. Additionally, an explanation of each equation used behind *Figure 8B* and the conversion from the theoretical continuity equation to the implementation of equations in Modelica is given in Annex 3 and Annex 5.

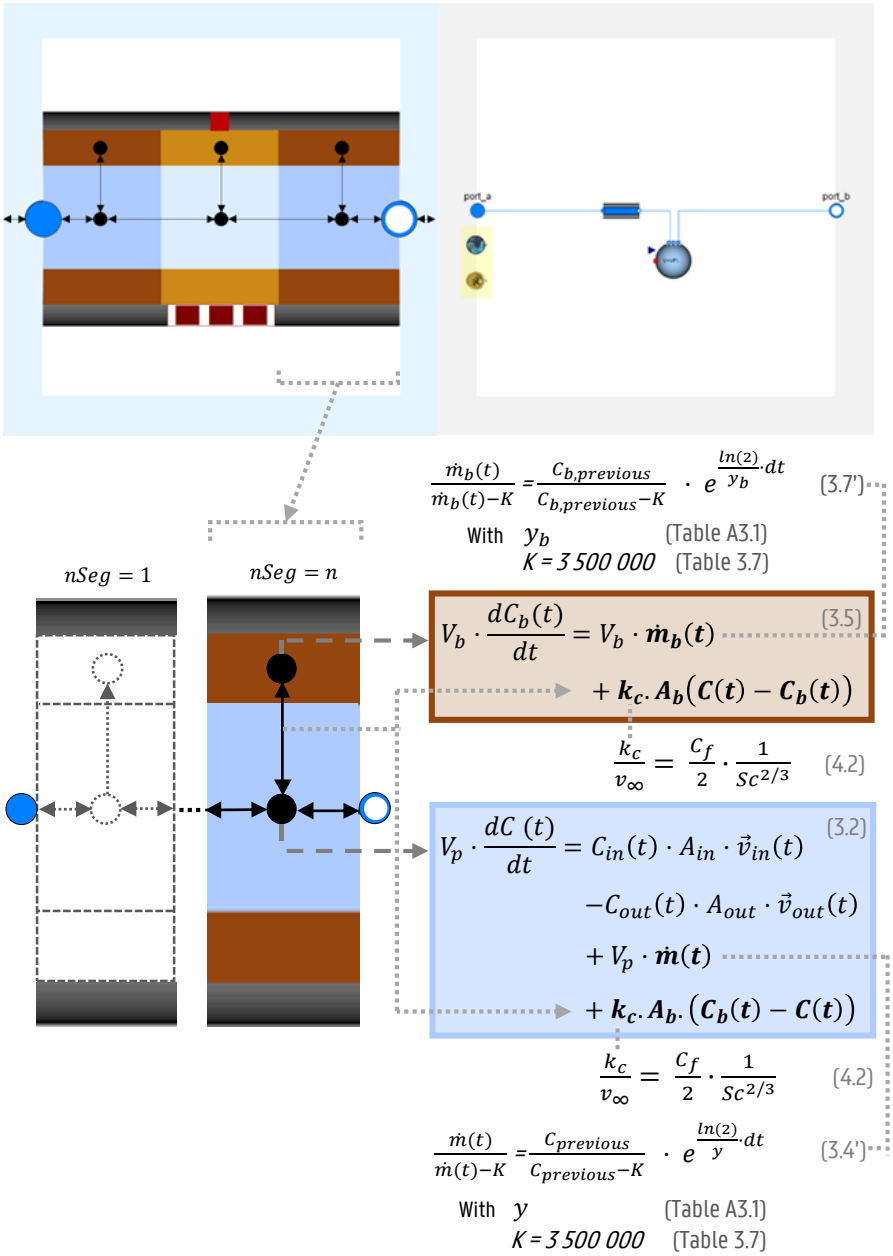

Figure 8. Customized Pipe model with addition of *L. pneumophila* growth equations A. Modelica icon view. B. Modelica diagram view with in yellow *L. pneumophila* growth equations (upper icon) and nutrients (lower icon).

Boiler model implementation

In the Buildings Fluid library, three model components are combined to make the StratifiedEnhancedInternalHex model, of which the second component is extended from the first, and the third from the second. As merely the second and third component are

used, the second component is adapted, and automatically the third component is adapted as this extends from the second one.

The modification of the retained StratifiedEnhancedInternalHex model (third component) from the Buildings (3.0.0) library can be seen in *Figure 9*. *Figure 9A* shows the visual representation of the customized model (icon view). The brown rectangles visually represent the addition of biofilm and the black circles the exchange of bacteria between biofilm and water. *Figure 9B* shows the thermohydraulic and biologic adaptation of the retained boiler model. *Equations 2-12* are written in this model (in yellow). *Figure 9B* is explained in more detail in *Annex 5 Table 11*. Additionally, an explanation of each equation used behind ***Error! Reference source not found.****B* and the conversion from the theoretical continuity equation to the implementation of equations in Modelica is given in *Annex 3* and *Annex 5*.

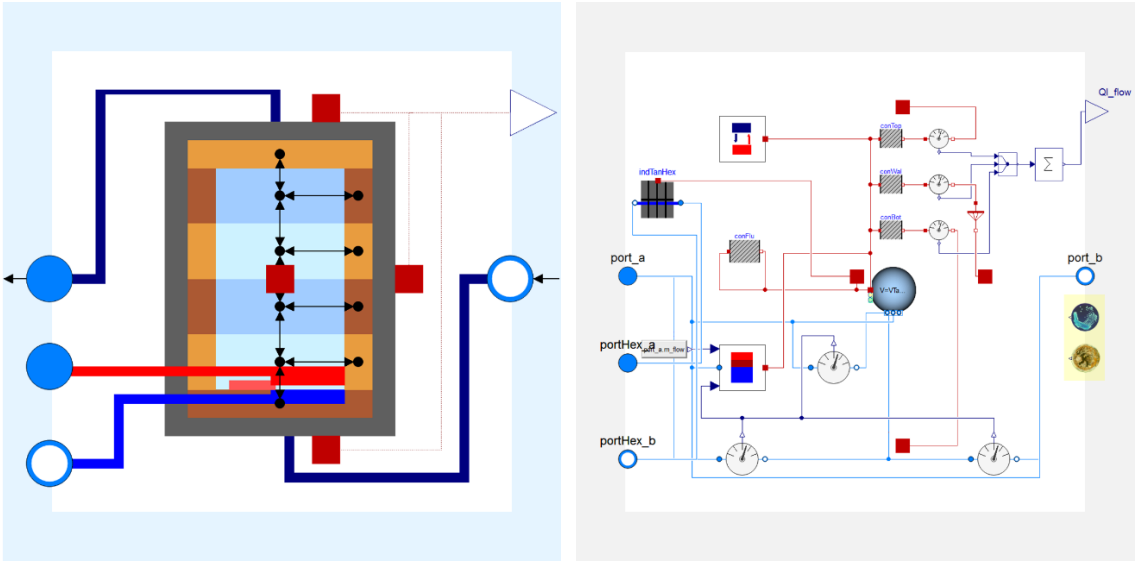

Figure 9. Customized StratifiedEnhancedInternalHex boiler model with addition of *L. pneumophila* growth equations. A. Modelica icon view. B. Modelica diagram view with in yellow *L. pneumophila* growth equations (upper icon) and nutrients (lower icon).

Computational costs

To give an indication of how the inclusion of the *L. pneumophila* model in the pipe and boiler element affects the numerical efficiency of the Modelica models, several aspects, such as the number of variables, number of time and state events and CPU time, are compared in *Table 4, 0* and *Table 6*. In *Table 4* the pipe and boiler component are used with and without the addition of the equations to calculate the *L. pneumophila* growth. Equations are divided into nontrivial and trivial equations. Trivial equations are simple equations from which you can immediately find the unknown. For nontrivial equations, a more difficult solution method must be applied (e.g., an iteration method). In *0* and *Table 6* the computational costs are presented for the pipe and the boiler component. More explanation to understand the simulation log basics is given in *Annex 6 Table 16*. The required solver is Euler because of the use of spatial and time discretization in the growth models. The simulation parameters used are:

- Solver Euler (explicit)
- Timestep 0.1s
- Tolerance 0.0001
- Number of pipe segments 2
- Number of boiler segments 8

Table 4. Statistical analyses of the pipe and boiler component model with and without *L. pneumophila* growth equations.

Number of…	**Pipe model without *Legionella***	**Pipe model with *Legionella***	**Difference**
Components	76	79	3
Variables	828	908	80
Constants	12	12	0
Parameters	388	421	33
Unknowns	428	475	47
Differentiated variables	14	18	4

Equations	339	376	37
Nontrivial	249	278	29
Trivial	90	103	13
Number of…	**Boiler model without *Legionella***	**Boiler model with *Legionella***	**Difference**
Components	172	176	4
Variables	2 160	2 256	96
Constants	31	31	0
Parameters	763	795	32
Unknowns	1 366	1 430	64
Differentiated variables	39	55	16
Equations	913	943	30
Nontrivial	669	686	23
Trivial	250	257	7

Table 5. Comparison of computational costs of the pipe component model with and without *L. pneumophila* growth equations.

Pipe model without *Legionella*		**Pipe model with *Legionella***	
CPU-time for integration	**16.9s**	**CPU-time for integration**	**39.9s**
CPU-time for one GRID interval	**0.90ms**	**CPU-time for one GRID interval**	**2.12ms**
Number of result points	189	Number of result points	189
Number of GRID points	189	Number of GRID points	189
Number of (successful) steps	564 000	Number of (successful) steps	564 000
Number of F-evaluations	564 000	Number of F-evaluations	564 000
Number of H-evaluations	564 001	Number of H-evaluations	564 005
Number of Jacobian-evaluations	0	Number of Jacobian-evaluations	0
Number of (model) time events	**56 399**	**Number of (model) time events**	**56 399**
Number of (U) time events	**0**	**Number of (U) time events**	**0**
Number of state events	**0**	**Number of state events**	**4**
Number of step events	**0**	**Number of step events**	**0**
Minimum integration stepsize	0.1	Minimum integration stepsize	0.1
Maximum integration stepsize	0.1	Maximum integration stepsize	0.1
Maximum integration order	1	Maximum integration order	1

Table 6. Comparison of computational costs of the boiler component model with and without *L. pneumophila* growth equations.

Boiler model without *Legionella*		**Boiler model with *Legionella***	
CPU-time for integration	**26.7s**	**CPU-time for integration**	**157s**
CPU-time for one GRID interval	**53.4ms**	**CPU-time for one GRID interval**	**2.79ms**
Number of result points	113 201	Number of result points	130 936
Number of GRID points	501	Number of GRID points	56 401
Number of (successful) steps	564 707	Number of (successful) steps	564 000
Number of F-evaluations	6 154 908	Number of F-evaluations	564 000
Number of H-evaluations	621 507	Number of H-evaluations	573 069
Number of Jacobian-evaluations	508 195	Number of Jacobian-evaluations	0
Number of (model) time events	**56 399**	**Number of (model) time events**	**56 399**
Number of (U) time events	**0**	**Number of (U) time events**	**0**
Number of state events	**0**	**Number of state events**	**9 068**
Number of step events	**0**	**Number of step events**	**0**

Minimum integration stepsize	0.0002	Minimum integration stepsize	0.1
Maximum integration stepsize	0.489	Maximum integration stepsize	0.1
Maximum integration order	2	Maximum integration order	1

Summary of simulation model assumptions

Although fragmentary mentioned throughout the paper, an overview of all simulation model assumptions is given below.

Component models assumptions

The three conservation equations are part of the DHW system component models (e.g., pipe, boiler): the law of conservation of mass (mass continuity equation), the first law of thermodynamics on energy conservation (energy equation) and Newton's second law of motion (momentum theorem) with pressure loss calculated with the Swamee-Jain equation, which is based on the Colebrook-White equation.

The *L. pneumophila* growth equations are added to the component models in the mass conservation equation. A dual control volume approach has been followed for water and biofilm. For the momentum and energy conservation equation, water and biofilm are considered as one node. This means that the temperature in the biofilm is assumed to be the same as the water temperature, which is correct for an insulated system. No separate velocity profile has been assumed in the biofilm.

The pipe model used is based on the finite volume method. Every pipe component is subdivided in nSeg nodes. Perfect mixing of water is assumed in every node. Flow reversal (back flow) is taken into account in the pipe model, based on pressure differences. Advection is included in two directions.

Diffusion between two water segments, in a pipe model and in between pipe models, is not taken into account in any Modelica pipe model as it is not part of the existing mass conservation equations in the underlying MixingVolume model in

Modelica. It should be possible to add this in future, but as for now reuse of the *L. pneumophila* model in different existing system component models is aimed for, meaning that it is necessary to use the existing mass conservation equation instead of replacing it in all components. Neglecting diffusion between different pipe segments can be done, as the model is used for systems with mainly continuous circulation, it is assumed that advection is much larger than diffusion. Only if stagnation occurs, diffusion can become important. Therefore an alternative T-section has been made to include diffusion from a distal pipe to the primary recirculation circuit. Diffusion between biofilm and water and thermal diffusion in the boiler are taken into account.

Water assumptions

The density of the medium is temperature dependent and the presence of *L. pneumophila* bacteria is not influencing the density of the mixture.

Nutrients *K* are coupled to the mass conservation equation, meaning that they are distributed by water flowing through the system, but no growth or decay equations for nutrients are coupled to this mass conservation equation. Nutrients are considered to be present in excess. This assumption is correct for systems with regular use, because a stock of nutrients is continuously entering the system. In reality, if water would stand still for a very long time, there would be no nutrient entering, meaning that *L. pneumophila* would die because of the lack of nutrients. However, literature confirms that *L. pneumophila* is found in systems without fresh nutrients after periods of two years (Garduno et al. 2002, Robertson et al. 2014, Al-Bana et al. 2014). If in future quantitative information on the relation between *L. pneumophila* and nutrients is available, it will be possible to add it to the model. However, in the current real system simulations with regular hot water use, the carrying capacity *K* is not reached by far, so a lower value of *K* would not change the results. In this case, the most critical situation

is modelled. Additionally, no active movement of bacteria based on nutrients is taken into account, meaning bacteria are not moving to areas with higher nutrient concentrations.

Biofilm assumptions

A fully grown biofilm is taken into account. The biofilm thickness is a parameter that cannot be measured easily. Based on discussions with biofilm experts (Biofilm conference, 2017), a cut-off value for the thickness has been assumed. The biofilm thickness is a function of the diameter of the pipe or boiler. The thickness of the biofilm is calculated based on the percentage of the volume. The biofilm thickness has been subtracted from the diameter to calculate the wall surface of a pipe or boiler. In the boiler, an extra condition has been added, namely that the thickness of biofilm on the bottom of the boiler is five times the thickness of the biofilm on the surface. If for a certain case the thickness of the biofilm would be known, it could be added to the model in one parameter.

The spatial structure of the biofilm is not taken into account due to the lack of literature data. Local vortexes are not taken into account, as the mass transfer coefficient kc is fixed. The mass transfer coefficient k_c between biofilm and water is function of the flow velocity and the concentration difference between biofilm and water.

A biofilm is thicker in pipes with a larger diameter, this can be explained by the speed profile in a pipe. The surface biofilm area of the boiler does not include the area of the heating elements inside. The volume of biofilm is considered to be divided over the wall's surface area. In future, it could be better to divide the volume over all surface elements.

Flow in between different biofilm segments is not taken into account, as literature shows that biofilms formed above 37°C have no water channels within (Mampel et al., 2006).

Result analysis

Proof of concept - simple domestic hot water system configuration

The Buildings (3.0.0) pipe and boiler model, with addition of *L. pneumophila* growth equations in water and biofilm, can now be used to build different DHW system configurations. The most simple system configuration is represented in *Figure 10*. This system contains a boiler with internal heat exchanger, the upper side of the boiler is connected to a pipe and a tap profile.

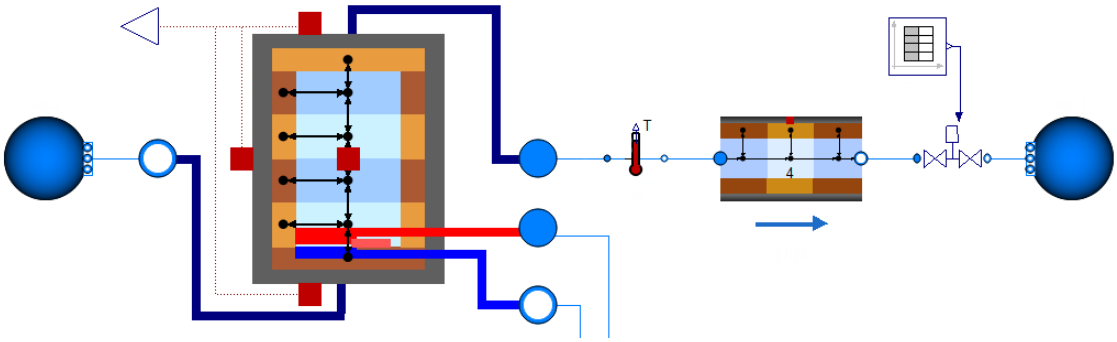

Figure 10. Simple DHW system with customized boiler and pipe components.

Initial model values are assigned to the biological parameters based on measurements, calculations, material characteristics and review of available literature. These parameter values are displayed in *Table 7*.

Table 7. Initial biological model parameter values (Brundrett 1992, Cervero-Aragó et al. 2015, Biofilm conference 2017, Van Kenhove et al. 2018)

Component	Modelling challenge	Parameter	Source for initial value	Initial model value
Boiler	Start concentration of *Legionella*	C_{start} [cfu/m³]	Cold water concentration	25

	Volume of biofilm	Volume [m³]	Literature review	$V_{tank}/10$
	Roughness	[m]	Material characteristics	Smooth steel: 0.000025
Pipes	Start concentration of *Legionella*	C_{start} [cfu/m³]	Cold water concentration	25
	Volume of biofilm	Volume [m³]	Literature review	$V_{pipe}/10$
	Roughness	[m]	Material characteristics	Smooth steel: 0.000025
Component independent	Mass transfer coefficient	[m/s]	Calculation	$k_c = \frac{C_f}{2} \cdot v_\infty$ Re < 3500: $C_f = \frac{1.328}{\sqrt{Re}}$ Re > 3500: $C_f = \frac{0.455}{\log(Re)^{2.58}}$
	Growth equation of *Legionella* in water	[cfu/m³]	Literature review	Water curve
	Growth equation of *Legionella* in biofilm	[cfu/m³]	Literature review + measurements	Biofilm curve
	Nutrients	[cfu/m³ => kg/m³]	Literature review + measurements	3 500 000 000

The hydraulic parameters which need to be defined by the user, are the same parameters as in the standard Pipe and StratifiedEnhancedInternalHex boiler model. Default values for these parameters are suggested by the developers of the Modelica components. The following parameter conditions are chosen to run the simulation of the system presented in *Figure 10*:

- length 20m (Length of pipe)
- diameter 0.05m (Diameter without insulation)
- dIns 0m (Insulation thickness of pipe)
- lambdaIns 0.026W/m·K (Lambda value of insulation)
- nSeg pipe 2 (Number of volume segments)
- nSeg boiler 8 (Number of volume segments)
- m_flow_nominal 0.0016kg/s (Nominal mass flow rate)
- dp_nominal 0.5Pa (Pressure difference)

The simulation setup is chosen as follows:

- start time 0s
- stop time 86 400s
- integration algorithm Euler (explicit)
- integration tolerance 0.0001
- timestep 0.1s

The simulation output is the following:

- Predicted *L. pneumophila* concentration in the pipe (pipe.vol[1].C) as in *Figure 11* (translated into *Figure 12* and *Figure 13*), *Figure 14* and *Figure 15*.
- Predicted *L. pneumophila* concentration at the outlet of the pipe (pipe.port_b.C_outflow[1]) as in *Figure 16*.

Verification exercise - reproducing growth time curves

To verify the growth time curves as in *Figure 2* (growth) and *Figure 3* (starvation), a similar temperature profile is imposed on the simulation model, namely a production temperature linearly rising from 25°C to 80°C. The predicted *L. pneumophila* concentration in *Figure 11* (concentration in function of temperature) is translated into *Figure 12* (growth-time curves). The predicted *L. pneumophila* concentrations in *Figure 12*, by simulating the system of *Figure 10*, show similar behaviour as in *Figure 2* and *Figure 3*. The same can be noticed from the growth/death curves of *L. pneumophila* in biofilm (*Figure 13*) based on the results of *Table 1*. RMSE of around 0 and R^2 of around 1 (cannot be expressed more accurately as the authors do not have the measurement data behind the curves, except from the visual appearance) are achieved between measurement points (black line) and simulation results (blue dotted line) because the measurement points are the inputs used in the component models.

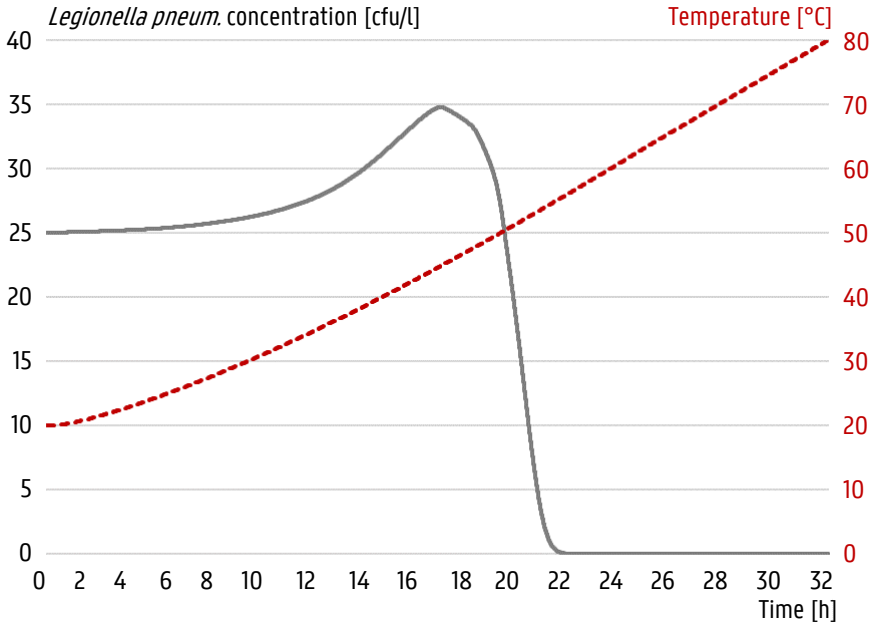

Figure 11. Predicted *L. pneumophila* concentration in pipe in function of outlet temperature.

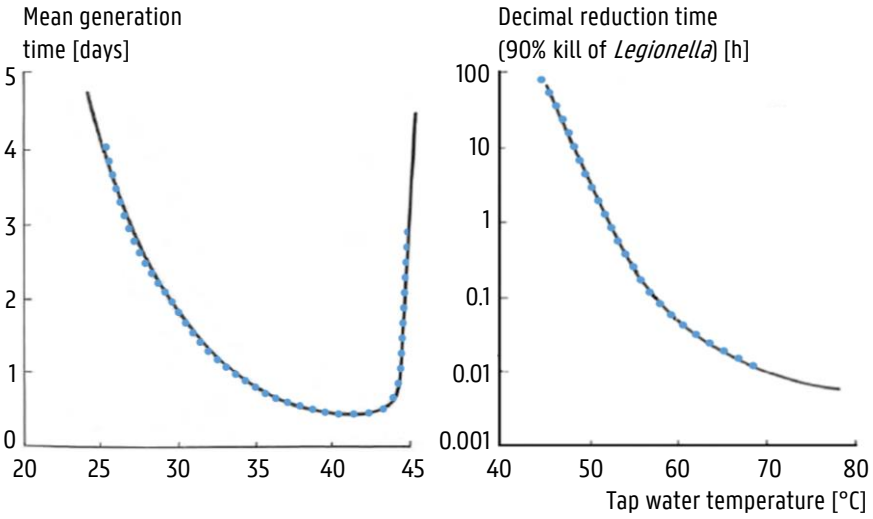

Figure 12. A. Simulation of mean generation time (time to double the number of cells) of *L. pneumophila* in water at different temperatures (blue dotted line: simulation result, black line: measurements from *Figure 2)*. B. Simulation of the change in decimal reduction time (90% reduction in *L. pneumophila* in water) at different temperatures (similar to *Figure 3*).

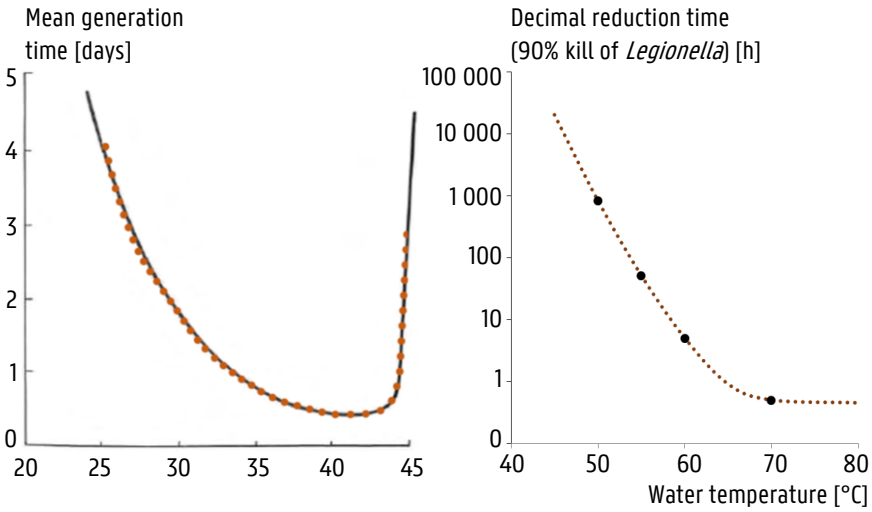

Figure 13. A. Simulation of mean generation time (time to double the number of cells) of *L. pneumophila* in biofilm (brown dotted line: simulation result, black line: measurements from *Figure 2*). B. Simulation of change in time to reduce 4 logs with temperature.

Sensitivity analyses

The robustness of the adapted component models is tested by running some simulations on the simple system presented in *Figure 10*, to assess the influence of several variables on the growth of *L. pneumophila.*

As seen before, *L. pneumophila* growth is dependent on temperature and mass flow rate. *Figure 14* shows the influence of the flow rate at a constant ideal growth temperature of 40°C. The biologic and hydraulic parameters are the same as before, only the mass flow rate is varied. A constant tap profile is implemented which is the same as the mass flow rate. *Figure 14* shows the concentration of *L. pneumophila* in the pipe for different velocities. As described in *equation 2*, the concentration of *L. pneumophila* is determined by three processes: mass flow of water through the pipe ($Q_{in}(t)$-$Q_{out}(t)$), temperature dependent growth of *L. pneumophila* in water ($\dot{m}(t)$) and mass transfer of *L. pneumophila* between biofilm and water (k_c). The mass transfer coefficient, used to calculate the mass transfer between biofilm and water will increase

with increasing velocity ($\frac{k_c}{v_\infty} = \frac{C_f}{2} \cdot \frac{1}{Sc^{2/3}}$). In case the velocity is zero or very small ($1e^{-6}$, $2e^{-6}$ and $2e^{-5}$kg/s), the concentration of *L. pneumophila* is mainly dependent on growth and mass transfer between biofilm and water. The influence of the incoming concentration ($C_{in}(t)$) (which is lower than the actual concentration in the pipe) is small. Compared to the case in which the mass flow is zero, a higher velocity ($1e^{-6}$, $2e^{-6}$ and $2e^{-5}$kg/s) results in a higher mass transfer between biofilm and water, resulting in a higher concentration *of L. pneumophila* in the pipe ($C(t)$). In case the velocity increases further, at a certain moment the influence of the incoming water with a low concentration of *L. pneumophila* ($C_{in}(t)$) becomes dominant over the growth ($\dot{m}(t)$) and mass transfer between biofilm and water ($k_c \cdot A_b \cdot (C_b(t) - C(t))$). Consequently, the concentration in the pipe decreases with increasing velocity. It can also be noted that the curve is S-shaped as expected. The growth is exponential until the carrying capacity *K* is reached, which is the same in all simulations, but as the flow rate becomes higher, it takes more time to reach *K*. At low velocities, a small amount of fresh water with a low concentration of *L. pneumophila* enters the pipe. As the flow rate becomes higher, more fresh water enters the pipe. Consequently, the higher the flow rate, the longer it takes for the *L. pneumophila* bacteria to reach the carrying capacity *K*. Dependent on the flow rate the carrying capacity is reached after 13 days or more.

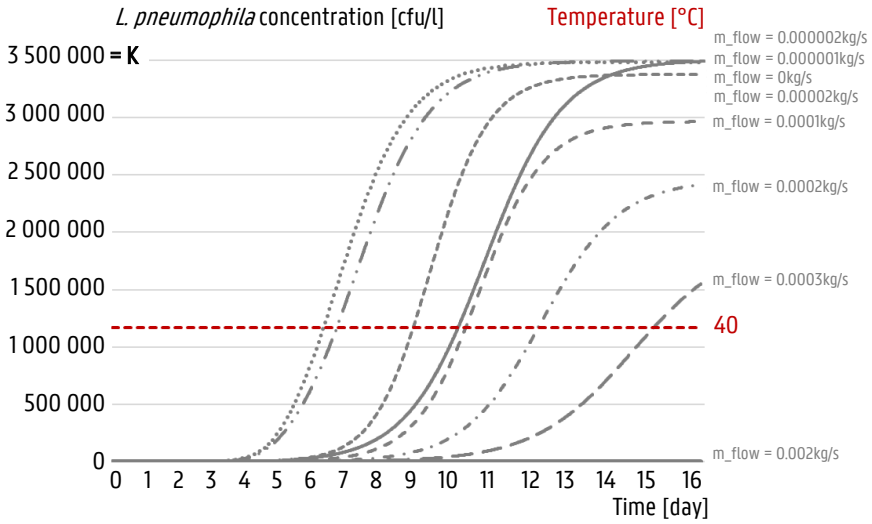

Figure 14. Influence of mass flow rate on *L. pneumophila* concentration at constant ideal temperature of 40°C over 16 days of simulation.

Figure 15 shows the influence of the insulation thickness on the temperature and the associated *L. pneumophila* growth over one day. Insulation is varied between 1cm, 2cm and 3cm, corresponding with a heat loss of the 20m long pipe of respectively 245W, 122W and 82W. The production temperature of the boiler is at constant 60°C, the temperature of the environment in the shaft is considered 30°C and the mass flow rate is 0.0016kg/s. A constant tap profile of 0.0016kg/s is added. Less insulation allows a drop into the critical temperature range, stimulating *L. pneumophila* growth. As can be seen on *Figure 15*, when 1cm insulation is present, a leap in the concentration curve can be noticed, this is due to the transition at < 45°C, causing growth in water. At higher temperatures the growth that can be noticed is caused by bacteria that are still growing in the biofilm and the mass transfer between biofilm and water.

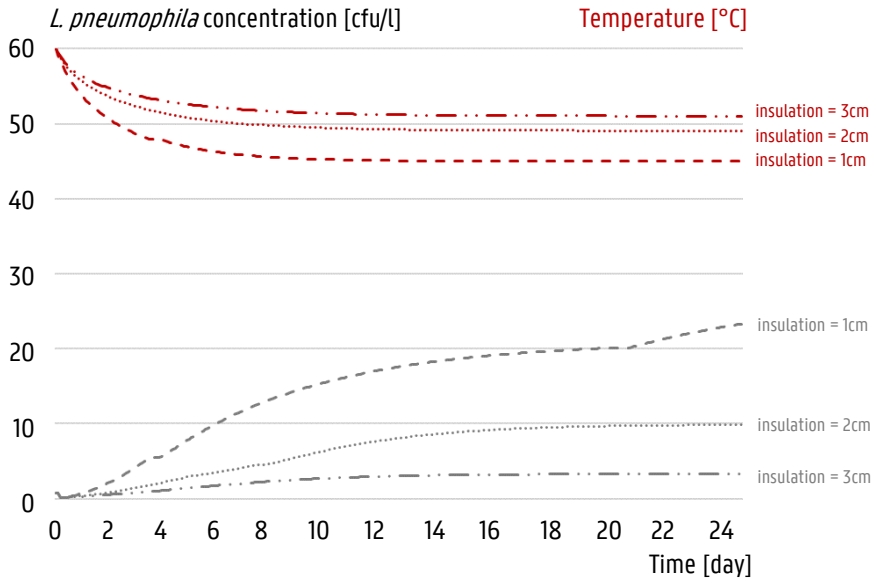

Figure 15. Influence of insulation on temperature and *L. pneumophila* concentration over simulation of 24 hours.

Also some numerical parameters are investigated. *Figure 16* shows the influence of the number of pipe volume segments on the *L. pneumophila* concentration. The boiler production temperature is linearly ascending from 0°C to 80°C (initial water temperature in pipe is 20°C). No pipe insulation is present. A variable tap profile is added, once every hour a tap with a duration of 10 minutes at a volume flow rate of 0.01l/s occurs. Pipe volume segments (length pipe/nSeg) are given lengths between 0.5 and 10m. The temperatures shown on the graph are the average temperatures in the first pipe segment. Only small differences in the results can be noted in pipe volume segment lengths up to 10m. The influence of the number of pipe volume segments on the *L. pneumophila* concentration results and on the calculation time is given in *Table 8*.

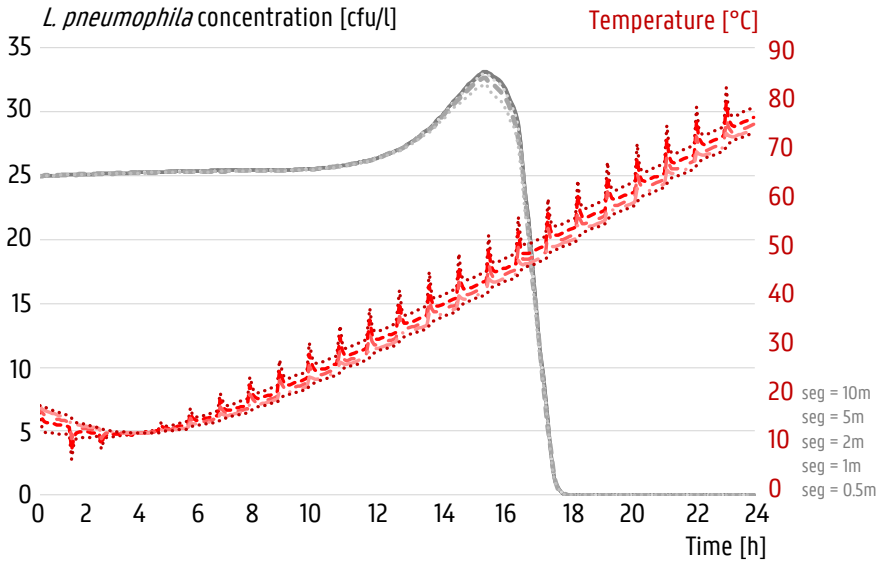

Figure 16. Influence of number of pipe volume segments on *L. pneumophila* concentration at different temperatures over 24 hours of simulation.

Table 8. Influence of number of pipe volume segments on *L. pneumophila* results [cfu/l] and calculation time [s].

Length of segment [m]	Number of segments	CPU-time for integration [s]	RMSE [cfu/l]
10	nSeg=2	21.9	0.3916
5	nSeg=4	39.2	0.1922
2	nSeg=10	100.0	0.0651
1	nSeg=20	201.0	0.02269
0.5	nSeg=40	406.0	0

Table 9 shows the influence of the chosen timestep on the results of the simple system model with a constant boiler production temperature of 40°C and no mass flow rate (stagnant water). No tap profile is added. RMSE [cfu/l] are calculated (compared with result of simulation with timestep of 0.001s).

In the results negligible differences in the *L. pneumophila* concentrations can be noted for timesteps up to 100s. It should however be said that the timestep can have an important influence on other parameters such as temperature. Additionally, if tap profiles with smaller time periods are added to the model, the timestep should be smaller than the smallest duration of one tap, to take all tap moments into account.

Table 9. Influence of timestep [s] on *L. pneumophila* results [cfu/l] and calculation time [s] for a simple system model at a constant 40°C with stagnant water.

Timestep [s]	CPU-time for integration [s]	RMSE [cfu/l]
100	0.015	0.07365
10	0.145	0.00737
2	0.826	0.00144
1	1.4	0.00073
0.1	21.8	0.0001
0.01	197	0.00006159
0.001	1990	0

Overall, the requirements set for the simulation model components are fulfilled. The combination of components can represent the DHW system of a building or parts of it. The modelling tool can estimate short-term *L. pneumophila* growth, as well as long-term growth (1s to 1 month). A timestep of 0.1-1s can be used and keeps the model fast enough. Higher timesteps up to 100s still produce sufficiently accurate *L. pneumophila* growth results in certain situations (e.g., stagnant water) and reduce the computation time by a factor between 100 and 1500. It is possible to perform the calculations on a 'standard' laptop (8GB RAM - CPU 2 cores - 2.67 GHz).

Taking it into practice

This was a first proof of concept to show that the *L. pneumophila* growth equations can be implemented in existing simulation components. In future, by further implementing the customized pipe and boiler model in more complex DHW system models, simulation results will allow to estimate the energy saving potential without increasing contamination risk. The questions that can be answered with the proposed simulation model are:

- By how much can we lower the DHW production temperature without compromising on comfort requirements (by simulating distribution heat losses)?

- Can we give a thermal shock of X°C every Y days during Z minutes to stay under the critical *L. pneumophila* concentration level and what are the X, Y and Z values for each case study DHW system?
- How much can we lower the DHW energy demand by reducing temperature without increasing contamination risk?

Discussion

The work performed in this paper has some limitations. For example, a fully developed biofilm is taken into account, this can result in an overestimation of the predicted *L. pneumophila* concentration when the system is used for the first time. The volume of biofilm is taken into account as a percentage of the pipe/boiler volume. In future research, this current simplification will be updated by making biofilm thickness function of the pipe's roughness and pipe sections (for example: more biofilm growth in pipe bends). It can also be an option in the future to take biofilm growth/decay (and its change in roughness) into account dynamically.

The assumption that the temperature of the biofilm is considered the same as the water temperature causes a limitation. This assumption is correct for well insulated systems but will deviate in uninsulated or poorly insulated systems.

The work performed in this paper could also be expanded in some ways. Firstly, the component models are validated based on growth curves. These growth curves are however conceived in laboratory conditions. The model will need to be further calibrated and validated dynamically based on DHW system measurements. This will be done in future research.

L. pneumophila transmission is caused by inhaling the aerosols from for example shower heads, however simulating the system contamination risk is chosen

over modelling the risk of aerosol inhalation. It is necessary to tackle the system contamination risk first. If *L. pneumophila* is not present in the system, it will be impossible to get contaminated by inhaling aerosols. For use in exposure studies, a model for aerosol formation and inhalation risk could be added to create a tool chain that can take the complete exposure pathway into account.

Conclusion

The energy use for the production, storage and distribution of DHW dominates the total energy use in well insulated and airtight buildings. Simulating *L. pneumophila* growth in DHW systems results in a more accurate prediction of the concentration of *L. pneumophila* in systems, which makes it possible to investigate energy saving alternatives without increasing contamination risk.

No previous research has been published on modelling *L. pneumophila* on DHW system level from a combined engineering-biological point of view.

After comparing different existing Modelica pipe and boiler models, those components are selected that are most compatible to the goals of this study and that could be extended to model *L. pneumophila* concentration in DHW. The Pipe model and the StratifiedEnhancedInteralHex models from the Buildings 3.0.0 library are retained.

Simulation model components are developed/updated that allow to investigate the contamination risk for *L. pneumophila* in a DHW system. The biological growth model is made up of a number of sub-equations: growth and transport of *L. pneumophila* in water, *L. pneumophila* growth in biofilm and bacteria transport between biofilm and water.

Some first proof of concept results are presented for a simple system application. Simulation of more realistic and extensive systems is part of future research. The first

proof of concept shows that the growth curves and equations can be translated into a dynamic simulation model responding to temperature and mass flow rate variations. The simulation results confirm that, if the mass flow rate is low, more *L. pneumophila* is present in the system, so stagnant areas are the most dangerous. Insulation should be added to the primary piping network to keep the temperatures out of the critical temperature range.

Additionally to the system conclusions, some simulation conclusions can be drawn. The length of one pipe volume segment can be up to 10m. No significant differences in concentration are seen for smaller pipe volume segment lengths. The smaller the timestep the more accurate the results, although for a timestep of 100s or less sufficient *L. pneumophila* results are obtained in certain situations.

By developing a simulation model that allows assessing the contamination risk for *L. pneumophila* in the design phase of a DHW system under dynamic conditions, HVAC designers will first be able to thoroughly assess the contamination risk associated with their design and secondly to optimise the temperature regimes, choose better hydronic controls and reduce the energy demand for DHW production.

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Nomenclature

$A(T)$	[-]	Growth function depending on water temperature, the species of the organism and the chemical nature of water
$B(T)$	[-]	Death function depending on water temperature, the species of the organism and the chemical nature of water
C_0	[cfu/m³]	Start concentration of *L. pneumophila* in water entering system
$C(t)$	[cfu/m³]	Concentration of *L. pneumophila* in water at time *t*
$C_{previous}$	[cfu/m³]	Concentration of *L. pneumophila* in water on previous timestep. $C_{previous} = C_0$ on first timestep.
$C_{in}(t)$	[cfu/m³]	Concentration of *L. pneumophila* in water entering system
$C_{out}(t)$	[cfu/m³]	Concentration of *L. pneumophila* in water leaving tap
$C_{b,in}(t)$	[cfu/m³]	Concentration of *L. pneumophila*. entering biofilm
$C_{b,out}(t)$	[cfu/m³]	Concentration of *L. pneumophila* in water leaving biofilm
$C_b(t)$	[cfu/m³]	Concentration of *L. pneumophila*. in biofilm at time *t*
$C_{b,previous}$	[cfu/m³]	Concentration of *L. pneumophila* in water on previous timestep. $C_{previous} = C_0$ on first timestep.
c_v	[J/kg·K]	Heat capacity
$dC(t)/dt$	[cfu/m³·s]	Changing concentration of *L. pneumophila* over time
$dC_b(t)/dt$	[cfu/m³·s]	Changing concentration of *L. pneumophila* in biofilm over time
D	[m]	Tube diameter
g	[m/s²]	Acceleration due to gravity
K	[cfu/m³]	Carrying capacity
k	[W/m·K]	Thermal conductivity

$\dot{m}(t)$	[cfu/m³·s]	Change in concentration of *L. pneumophila*. due to growth or starvation
$\dot{m}_b(t)$	[cfu/m³·s]	Change in concentration of *L. pneumophila* in biofilm due to growth or starvation
P	[Pa]	Total pressure
$Q_{in}(t)$	[kg/s]	Mass flow rate of *L. pneumophila* in water entering system
$Q_{out}(t)$	[kg/s]	Mass flow rate of *L. pneumophila* in water leaving tap
$Q_b(t)$	[kg/s]	Mass flow rate of *L. pneumophila* entering/leaving biofilm
$\dot{q}$	[W/m³]	Volumetric energy generation rate
t	[s]	Time
T	[K]	Absolute temperature
V_p	[m³]	Volume of water in pipe
V_b	[m³]	Volume of biofilm in pipe
y	[s]	Multiplication time of *L. pneumophila* in water dependent on temperature
y_b	[s]	Multiplication time of *L. pneumophila* in biofilm dependent on temperature
v	[m/s]	Mass-average velocity for multicomponent mixture
μ	[Pa·s]	Viscosity
ρ	[kg/m³]	Mass density of mixture
Φ		Function of fluid viscosity and shear strain rates

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Attachment

Annex 1 - ***Approach 1 to determine multiplication time (y and y_b)***
Annex 2 - ***Approach 2 to determine multiplication time (y and y_b)***
Annex 3 - ***Explanation of conservation equations***
Annex 4 - ***Pipe and boiler models: reasons for non-retention***
Annex 5 - ***Simulation model components used in pipe and boiler component***
Annex 6 - ***Understanding the simulation log basics***

Annex 1 - ***Alternative approach to determine multiplication time (y and y_b)***

More explanation alternative approach

The rate of increase of *L. pneumophila* in **water** is temperature dependent. Because it is necessary to know the growth rate at every timestep, a function is created in Modelica which returns the growth rate *y*. Growth coefficient *y* is a time constant [s] to predict growth or death of *L. pneumophila* in water. *y* in *Equation 4* is dependent on water temperature *T* in the pipe or boiler component. y_2 (time to reduce *L. pneumophila* with 90%, 10% remains) is rewritten as a negative mean generation time to express only one *y*-value. Equations of *y* are made for *L. pneumophila* in water, based on piece-wise fitting of the curve presented in literature in *Figure 2* and *Figure 3*. The chosen function is based on the behaviour of the curve in the determined temperature region (linear, polynomial and constant) (*Equation 9*).

$$
\begin{aligned}
&T \leq 20°C && y = 1\,000\,000 \\
&20°C < T < 25°C && y = -128\,996.48 \cdot T + 3\,579\,929.60 \\
&25°C \leq T < 44°C && y = 2.9988090226 \cdot T4 - 473.8259729333 \cdot T3 \\
& && \quad +28\,717.2386165937 \cdot T2 - 793\,367.9422568690 \cdot T \\
& && \quad +8\,473\,063.073695 \\
&44°C \leq T < 45°C && y = 230\,040 \cdot T - 10\,082\,880 \\
&45°C \leq T < 48°C && y = -4.62917026659765 \cdot 1036 \cdot T - 20.5367087417573 \\
&48°C \leq T < 70°C && y = -4.62917026727924 \cdot 1039 \cdot T - 20.5367087418 \\
&70°C \leq T < 80°C && y = 5.53698974855826 \cdot T - 501.797170301305 \\
&T \geq 80°C && y = -58.8512781290245
\end{aligned}
\qquad (9)
$$

Growth coefficient y_b is a function to predict growth or death of *L. pneumophila* in **biofilm**. y_b in *Equation 7* is dependent on water temperature *T* in the pipe or boiler component. y_b was originally split up in y_3, y_4 and y_5. y_3 is the mean generation time in biofilm (time to double the number of cells), y_4 is the decimal reduction time in biofilm (time to reduce *L. pneumophila* with 90%, 10% remains) and y_5 is the 4 log reduction time in biofilm (time to reduce *L. pneumophila* with 99.99%, 0.01% remains). Growth coefficient y_5 is added for growth of *L. pneumophila* in biofilm based on the results of Cervero-Aragó (2015). y_4 and y_5 are rewritten as negative mean generation times to express only one *y*-value. *Equation 10* are the equations of y_b for *L. pneumophila* in biofilm, based on piece-wise fitting of the curve and measurement points presented in literature in *Figure 2* and *Table 1*. The chosen function is based on the behavior of the curve in the determined temperature region (linear, polynomial and constant).

$T \leq 20°C$ $\quad y_b = 1\ 000\ 000$

$20°C < T < 25°C$ $\quad y_b = -128\ 996.48 \cdot T + 3\ 579\ 929.60$

$25°C \leq T < 44°C$ $\quad y_b = 2.9988090226 \cdot T^4 - 473.8259729333 \cdot T^3 + 28\ 717.2386165937 \cdot T^2 - 793\ 367.9422568690 \cdot T + 8\ 473\ 063.073695$

$44°C \leq T < 45°C$ $\quad y_b = 393\ 120 \cdot T - 17\ 258\ 400$

$45°C \leq T < 50°C$ $\quad y_b = -1.30591637266212 \cdot 10^6 \cdot T - 5.73311638328041 \cdot 10^7$

$50°C \leq T < 70°C$ $\quad y_b = -6.16712951164611 \cdot 10^{42} \cdot T^{-21.8803778292}$

$70°C \leq T < 80°C$ $\quad y_b = 22.147958994233 \cdot T - 2007.18868120522$

$T \geq 80°C$ $\quad y_b = -235.405112516098$ *(10)*

Original functions alternative approach

To model *L. pneumophila* growth in **water** in a pipe *Equation 4* was originally split up in *Equation 4A* and *4B.*

$$\dot{m}(\mathrm{t}) = C_{previous} \cdot \frac{ln(2)}{y1} \cdot e^{\frac{ln(2)}{y1} \cdot dt} (\text{growth}) \quad (4A)$$

$$\dot{m}(t) = C_{previous} \cdot \frac{ln(1/10)}{y2} \cdot e^{\frac{ln(1/10)}{y2} \cdot dt} (\text{death}) \quad (4B)$$

Growth coefficients y_1 *and* y_2 are time constants [s] to predict growth (y_1) or death (y_2) of *L. pneumophila* in water. y_1 in *Equation 4A* and y_2 in *Equation 4B* are dependent on the temperature *T* of water in the pipe component. y_1 is the mean generation time in water (time to double the number of cells), y_2 is the decimal reduction time in water (time to reduce *L. pneumophila* with 90%, 10% remains). y_1 is the mathematical translation of *Figure 2* and y_2 of *Figure 3*. Equations of y_1 and y_2 are made for *L. pneumophila* in water based on curve fitting (*Equation 11*).

$T \leq 20°C$ $\quad y_1 = 1\ 000\ 000$

$20°C < T < 25°C$ $\quad y_1 = -128\ 996.48 \cdot T + 3\ 579\ 929.60$

$25°C \leq T < 44°C$ $\quad y_1 = 2.9988090226 \cdot T^4 - 473.8259729333 \cdot T^3 + 28\ 717.2386165937 \cdot T^2 - 793\ 367.9422568690 \cdot T$

$+8\ 473\ 063.073695$

44°C ≤ T < 45°C $y_1 = 230\ 040 \cdot T - 10\ 082\ 880$

45°C ≤ T < 48°C $y_2 = 139\ 351\ 910\ 528\ 172 \cdot 10^{25} \cdot T^{-20.5367087417573}$

48°C ≤ T < 70°C $y_2 = 13\ 935\ 191\ 054\ 869 \cdot 10^{26} \cdot T^{-20.5367087418}$

70°C ≤ T < 80°C $y_2 = -1.6668 \cdot T + 151.056$

T ≥ 80°C $y_2 = 17.716$ (11)

To model *L. pneumophila* growth in **biofilm** in a pipe *Equation 7* was originally split up in *Equation 7A*, *7B* and *7C*.

$$\dot{m}_b(\mathrm{t}) = C_{\mathrm{b,previous}} \cdot \frac{ln(2)}{y3} \cdot e^{\frac{ln(2)}{y3} \cdot dt} \text{(growth)} \quad (7A)$$

$$\dot{m}_b(\mathrm{t}) = C_{\mathrm{b,previous}} \cdot \frac{ln(1/10)}{y4} \cdot e^{\frac{ln(1/10)}{y4} \cdot dt} \text{(death)} \quad (7B)$$

$$\dot{m}_b(\mathrm{t}) = C_{\mathrm{b,previous}} \cdot \frac{ln(1/10{,}000)}{y5} \cdot e^{\frac{ln(1/10{,}000)}{y5} \cdot dt} \text{(death)} \quad (7C)$$

Growth coefficients y_3, y_4 *and* y_5 are functions to predict growth (y_3) or death (y_4, y_5) of *L. pneumophila* in biofilm. y_3 in *Equation 7A*, y_4 in *Equation 7B* and y_5 in *Equation 7C* are dependent on the temperature *T* of water in the pipe component. y_3 is the mean generation time in biofilm (time to double the number of cells), y_4 is the decimal reduction time in biofilm (time to reduce *L. pneumophila* with 90%, 10% remains) and y_5 is the 4 log reduction time in biofilm (time to reduce *L. pneumophila* with 99.99%, 0.01% remains). Growth coefficient y_5 is added for growth of *L. pneumophila* in biofilm based on the results of Cervero-Aragó (2015). *Equation 12* are the equations of y_3, y_4 and y_5 for *L. pneumophila* in biofilm.

T ≤ 20°C $y_3 = 1\ 000\ 000$

20°C < T < 25°C $y_3 = -128\ 996.48 \cdot T + 3\ 579\ 929.60$

25°C ≤ T < 44°C $y_3 = 2.9988090226 \cdot T^4 - 473.8259729333 \cdot T^3 + 28\ 717.2386165937 \cdot T^2 - 793\ 367.9422568690 \cdot T + 8\ 473\ 063.073695$

44°C ≤ T < 45°C $y_3 = 393\ 120 \cdot T - 17\ 258\ 400$

45°C ≤ T < 50°C $y_4 = 393\ 120 \cdot T - 17\ 258\ 400$

50°C ≤ T < 70°C $y_5 = 46\ 412\ 274\ 253\ 751 \cdot 10^{28} \cdot T^{-21.8803778292}$

70°C ≤ T < 80°C $y_5 = -1.6668 \cdot T + 151.056$

T ≥ 80°C $y_5 = 17.716$ (12)

To take K into account equation 4A, 4B, 7A, 7B and 7C become respectively 4A', 4B', 7A', 7B' and 7C'.

$$\frac{\dot{m}(t)}{\dot{m}(t)-K} = \frac{C_{previous}}{C_{previous}-K} \cdot e^{\frac{ln(2)}{y_1} \cdot dt} \quad (4A')$$

$$\frac{\dot{m}(t)}{\dot{m}(t)-K} = \frac{C_{previous}}{C_{previous}-K} \cdot e^{\frac{ln(1/10)}{y_2} \cdot dt} \quad (4B')$$

$$\frac{\dot{m}_b(t)}{\dot{m}_b(t)-K} = \frac{C_{b,previous}}{C_{b,previous}-K} \cdot e^{\frac{ln(2)}{y_3} \cdot dt} \quad (7A')$$

$$\frac{\dot{m}_b(t)}{\dot{m}_b(t)-K} = \frac{C_{b,previous}}{C_{b,previous}-K} \cdot e^{\frac{ln(1/10)}{y_4} \cdot dt} \quad (7B')$$

$$\frac{\dot{m}_b(t)}{\dot{m}_b(t)-K} = \frac{C_{b,previous}}{C_{b,previous}-K} \cdot e^{\frac{ln(1/10{,}000)}{y_5} \cdot dt} \quad (7C')$$

This alternative approach gives the same results as the finally used approach.

Annex 2 - *Finally used approach to determine multiplication time (y and y_b)*

In the finally used approach, the function is organized differently by fitting a polynomial through the defined points in Modelica, i.e., a vector containing temperature points and a vector containing the corresponding multiplication time of *L. pneumophila.* The points are the same as in the alternative approach, determined from literature, used with an interval of 1K as shown in *Table 10*.

Table 10. Temperature and *L. pneumophila* concentration multiplication time points.

***T* [°C]**	***y* [s]**	***y_b* [s]**
20	1000000.0	1000000.0
21	905191.0	905191.0
22	767170.0	767170.0
23	612057.0	612057.0
24	465967.0	465967.0
25	355018.0	355018.0
26	284428.0	284428.0
27	236787.0	236787.0
28	204267.0	204267.0
29	179038.0	179038.0
30	153274.0	153274.0

31	127981.0	127981.0
32	108379.0	108379.0
33	92956.7	92956.7
34	80201.3	80201.3
35	68601.6	68601.6
36	58904.6	58904.6
37	52118.2	52118.2
38	47121.7	47121.7
39	42794.5	42794.5
40	38016.0	38016.0
41	38100.0	38100.0
42	38200.0	38200.0
43	41000.0	41000.0
44	55000.0	38880.0
45	250000.0	-116097400.6
45	-80953.0	-116097400.6
46	-51175.0	-117403317.0
47	-30103.0	-118709233.3
48	-16557.0	-120015149.7
49	-8127.8	-121321066.1
50	-4263.0	-413026.0591
51	-2408.2	-267794.9888
52	-1384.7	-175098.1485
53	-782.68	-115418.5357
54	-451.54	-76674.87117
55	-301.03	-51320.37993
56	-180.62	-34599.39632
57	-123.42	-23489.71816
58	-90.309	-16055.07339
59	-67.732	-11045.15906
60	-52.17	-7646.485565
61	-42.144	-5325.884319
62	-34.618	-3731.433315
63	-28.297	-2629.250731
64	-24.082	-1862.871123
65	-20.771	-1326.947846
66	-18.643	-950.1108603
67	-17.378	-683.7170992
68	-15.879	-494.4196052
69	-13.114	-359.2280101
70	-10.349	-456.8315516
71	-9.8477	-434.6835926
72	-9.3459	-412.5356336
73	-8.8441	-390.3876746

74	-8.3424	-368.2397156
75	-7.8406	-346.0917566
76	-7.3389	-323.9437976
77	-6.8371	-301.7958386
78	-6.3354	-279.6478797
79	-5.8336	-257.4999207
80	-5.3318	-235.4051125

Annex 3 - ***Explanation of conservation equations***

Continuity equation

A continuity equation is an equation that describes the transport of some quantity. The majority of physical phenomena can be described using continuity equations, e.g., mass, energy and momentum as they are conserved under their respective appropriate conditions. The differential form of the continuity equation is *Equation 13*.

$$\frac{\partial}{\partial t}\rho + \nabla j = \dot{s} \tag{13}$$

With:

- ρ [kg/m³] Amount of quantity q per unit volume (density)
- j Flux of q
- $\dot{s}$ Source or sink

Conservation of mass (medium: water with L. pneumophila)

In Fluid Dynamics, the mass conservation equation states that the rate at which mass enters a system is the rate at which it leaves the system: $\nabla\rho \cdot \vec{v}$ summed with the accumulation of mass within the system: $\frac{\partial}{\partial t}\rho$. The differential form of the mass conservation equation is *Equation 14*.

$$\frac{\partial}{\partial t}\rho + \nabla\rho \cdot \vec{v} = 0 \tag{14}$$

With:

- ρ [kg/m³] Amount of quantity q per unit volume (density)
- $\vec{v}$ [m/s] Velocity

Converting this equation to 1D gives *Equation 15*.

$$\Leftrightarrow \frac{\partial}{\partial t}\rho + \rho \cdot \frac{\partial}{\partial x} v_x = 0 \tag{15}$$

The integral form of this equation is *Equation 16*.

$$\Leftrightarrow \iiint \frac{\partial}{\partial t}\rho \cdot dV = \iint \frac{\partial}{\partial x} v_x \cdot dA \tag{16}$$

Solving this integral gives *Equation 17*.

$$\Leftrightarrow V \cdot \frac{d\rho}{dt} = \rho_{in} \cdot v_{in} \cdot A_{in} - \rho_{out} \cdot v_{out} \cdot A_{out} \tag{17}$$

Conservation of energy (medium: water with L. pneumophila)

The law of conservation of energy states that energy can neither be created nor destroyed. This law is combined with the First Law of Thermodynamics, which states that, although energy cannot be created or destroyed, it can be transformed or transferred from one form to another. This results in the energy conservation equation, stating that the rate of change of energy inside the fluid element $\rho \cdot \frac{\partial}{\partial t} u$, with $u = C \cdot T$, is the net flux of heat into the element (conduction component $\frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right)$) and transport component $\rho \cdot v_x \cdot \frac{\partial}{\partial x} u$ summed with the rate of working done on the element due to body and surface forces $\dot{q} + \Phi$. The differential form of the energy conservation equation is *Equation 18.*

$$\frac{\partial}{\partial t}\rho \cdot u + \nabla \rho \cdot \overrightarrow{v \cdot u} = -\nabla q_c + \dot{q} + \Phi \tag{18}$$

With:

- u [J] Internal energy
- q_c [W/m²] Conduction of heat, equal to $\nabla k \cdot \nabla T$
- $\dot{q}$ [W/m³] Heat source
- Φ [W/m³] Heat losses due to friction and pressure losses

Converting this equation to 1D gives *Equation 19*.

$$\Leftrightarrow \rho \cdot \left(\frac{\partial}{\partial t} u + v_x \cdot \frac{\partial}{\partial x} u\right) = \frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right) + \dot{q} + \Phi \tag{19}$$

Modelica works with enthalpy in the heat flux equation $\rho \cdot v_x \cdot \frac{\partial}{\partial x} u$. Knowing that the enthalpy is $h = u + \frac{P}{\rho}$, if water is incompressible $h = c_p \cdot T$.

The integral form of this equation becomes *Equation 20*.

$$\Leftrightarrow \iiint \frac{\partial}{\partial t} \rho \cdot u \cdot dV = \iint \frac{\partial}{\partial x} v_x \cdot h \cdot dA + \iint \frac{\partial}{\partial x} \left(k \cdot \frac{\partial T}{\partial x} \right) \cdot dA + \iiint \dot{q} \cdot dV + \iiint \Phi \cdot d \quad (20)$$

Solving this integral gives *Equation 21*.

$$\Leftrightarrow \rho \cdot V \cdot \left(\frac{d}{dt} u \right) = \rho \cdot v_{in} \cdot A_{in} \cdot h_{in} + \rho \cdot v_{out} \cdot A_{out} \cdot h_{out} + Q_{cond} + Q_{source} + Q_{diss} \quad (21)$$

Momentum conservation (medium: water with L. pneumophila)

The Momentum equation in Modelica is integrated in the form of the Navier-Stokes equation, which results from Newton's second law, stating that $F = m \cdot a$. The Navier-Stokes equation states that the mass, multiplied by the acceleration of fluid particles, is proportional to the forces (volume forces and surface forces) acting on them. The differential form of the momentum equation is *Equation 22*.

$$\frac{\partial}{\partial t} \rho \cdot v + \nabla \rho \cdot \overrightarrow{v \cdot v} = \rho \cdot g - \nabla P + \nabla \tau \quad (22)$$

Converting this equation to 1D gives *Equation 23*.

$$\Leftrightarrow \rho \cdot \left(\frac{\partial}{\partial t} v_x + v_x \cdot \frac{\partial}{\partial x} v_x \right) = \rho \cdot g_x - \frac{\partial P}{\partial x} + \nabla (\mu \cdot \nabla v_x) \quad (23)$$

The integral form of this equation is *Equation 24*.

$$\Leftrightarrow \frac{\partial}{\partial t} \iiint \vec{v} \cdot \rho \cdot dV = \iint v \cdot (\rho(\vec{v}) \cdot dA + \rho \cdot g_x - \frac{\partial P}{\partial x} + \nabla (\mu \cdot \nabla v_x) \quad (24)$$

Solving this integral gives *Equation 25*.

$$\Leftrightarrow \rho \cdot V \cdot \frac{d\vec{v}}{dt} = \rho \cdot v_{in}^2 \cdot A_{in} - \rho \cdot v_{out}^2 . A_{in} + \rho \cdot g_x - \frac{dP}{dx} + \nabla (\mu \cdot \nabla v_x) \quad (25)$$

This equation can be simplified to a pressure-based equation based on Bernoulli (*Equation 26*).

$$\Leftrightarrow 0 = \frac{{v_2}^2}{2g} - \frac{{v_1}^2}{2g} + (h_2 - h_1) + (\frac{P_2}{\rho g} - \frac{P_1}{\rho g}) + (\Delta h_f + \Delta h_m + \Delta h_p) \quad (26)$$

With:

- Δh_p Pressure rise by pump
- Δh_f Major losses (in relation to length of pipe)
- Δh_m Minor friction losses (e.g., fittings)
- 1 Entrance port
- 2 Exit port

Trace substance equation of L. pneumophila

The principle of the conservation equation for *L. pneumophila* concentration is based on the principle of conservation of mass. *Equation 2* and *Equation 5* are coming from the following equations. The differential form of the trace substance equation is *Equation 27*.

$$\frac{\partial}{\partial t} C + \nabla C \cdot \vec{v} = \dot{C} \tag{27}$$

With:

- C Total number of bacteria (cfu) per unit mixture volume (water with bacteria)
- $\dot{C}$ Source and sink, this is the growth of *L. pneumophila* in water and the mass transfer between water and biofilm

Converting this equation to 1D gives *Equation 28*.

$$\Leftrightarrow \frac{\partial}{\partial t} C + \frac{\partial}{\partial x} C \cdot v_x = \dot{C} \tag{28}$$

The integral form of this equation is *Equation 29*.

$$\Leftrightarrow \iiint \frac{\partial}{\partial t} C \cdot dV = \iint \frac{\partial}{\partial x} \cdot C \cdot v_x \cdot dA + \dot{C} \tag{29}$$

Solving this integral gives *Equation 30*.

$$\Leftrightarrow V \cdot \frac{dC}{dt} = C_{in} \cdot v_{in} \cdot A_{in} - C_{out} \cdot v_{out} \cdot A_{out} + \dot{C} \tag{30}$$

With: $\dot{C} = V_p \cdot \dot{m}(t) + k_c \cdot A_b \cdot (C_b(t) - C(t))$ in *Equation 2*.

Mass, momentum and energy conservation equation parameters to compare different pipe and boiler models

Mass conservation: $\frac{\partial}{\partial t}\rho + \rho \cdot \frac{\partial}{\partial x} v_x = 0$ (31)

- Trace substances ρ

Can be solved by one node for the whole component, or the component can be split into a number of nodes (nNodes).

Momentum conservation: $\frac{\partial}{\partial \mathrm{t}} v_x + v_x \cdot \frac{\partial}{\partial \mathrm{x}} v_x = \rho \cdot g_x - \frac{\partial P}{\partial x} + \nabla(\mu \cdot \nabla v_x)$ (32)

- Gravity $\rho \cdot g_x$
- Pressure drop $\frac{\partial P}{\partial x}$
- Laminar/turbulent flow $\frac{\partial P}{\partial x}$ or $\nabla(\mu \cdot \nabla v_x)$
- Friction/material roughness $\nabla(\mu \cdot \nabla v_x)$

Energy conservation: $\left(\frac{\partial}{\partial t} u + v_x \cdot \frac{\partial}{\partial x} u\right) = \frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right) + \dot{q} + \Phi$ (33)

- Heat source $\dot{q}$
- Heat exchange/insulation $\frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right)$
- nNodes $\frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right)$

With:

- c_p [J/kg·K] Heat capacity, used to calculate *u*
- g_x [m/s²] Acceleration due to gravity
- k [W/m·K] Thermal conductivity
- P [Pa] Total pressure
- $\dot{q}$ [W/m³] Volumetric energy generation rate
- t [s] Time
- T [K] Absolute temperature
- $\vec{v}$ [m/s] Mass-average velocity for multicomponent mixture (velocity split up in v_x, v_y and v_z)
- μ [Pa·s] Viscosity
- ρ [kg/m³] Mass density of mixture
- ∇ Partial derivative to x-, y- and z-direction, $(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z})$

Annex 4 - *Pipe and boiler models: reasons for non-retention*

Pipe models

Out of the comparison of the different pipe models in *Table 2*, there are four models suitable for the authors' applications.

- Dynamic pipe: Dynamic pipe model with storage of mass and energy (Modelica 3.2.1)
- Insulated pipe: Insulated pipe characterized by a UA value (OpenIDEAS 0.3.0)

- Pipe insulated: Pipe with insulation, characterized by UA (OpenIDEAS 0.3.0)
- Pipe: Pipe with finite volume discretization along flow path (Buildings 3.0.0)

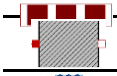
'Dynamic pipe' model was not chosen for further development because insulation of the pipe has not been taken into account in the standard model. 'Insulated pipe' and 'Pipe Insulated', two very similar models, cannot be divided into smaller pipe volume segments (nNodes). Moreover, material roughness, a parameter that is important to simulate biofilm formation, is not taken into account. That is the reason why these models were not retained.

Boiler models

'Boiler' and 'OpenTank' model were not chosen for further development because insulation of the boiler has not been taken into account in the model. Although insulation could easily be implemented if these models need to be used for this application in future. Additionally these models and 'Boiler polynomial' cannot be divided into smaller pipe volume segments (nNodes). In the 'OpenTank' and 'Storage Tank' model the addition of a heat source is not possible. 'StorageTank_OneIntHex' is not chosen because of the impossibility to add trace substance and the lack of pressure drop and laminar/turbulent flow equations.

Annex 5 - *Simulation model components used in pipe and boiler component*

Table 11. Explanation of simulation model components used in the pipe and boiler components.

Component	Information
	Generic fluid connector at design inlet for quasi one-dimensional fluid flow in a piping network (incompressible or compressible, one or more phases, one or more substances)
	Generic fluid connector at design outlet for quasi one-dimensional fluid flow in a piping network (incompressible or compressible, one or more phases, one or more substances)
	Collects the heat flows from m heatports to one single heatport
	Fixed flow resistance with dp and m_flow as parameter
	Connector used for 1-dimensional heat flow between components
	HeatPort connector to be used for vectors of HeatPorts (vector dimensions must be added after dragging)
	Lumped thermal element transporting heat without storing it
	Mixing volume with inlet and outlet ports (flow reversal is allowed) with heat port
	Heat exchanger typically submerged in a fluid with a second fluid circulating through it
	Model to add buoyancy, if there is a temperature inversion in the tank
	Model to reduce the numerical dissipation that is introduced by the standard first-order upwind discretization scheme, which is created when connecting fluid volumes in series
	Ideal enthalpy mass flow rate sensor
	Multiplexer block for three input connectors
	Outputs the sum of the elements of the input vector
	Output ‘Real' as connector

Conversion from theoretical continuity equation (*Annex 3*) to implementation of equations in Modelica Buildings library

Mass and energy conservation equation

The conservation equations are implemented in Buildings Fluid Library under the following form (*Comparison of theoretical mass and energy equation and implementation in* Modelica.).

Table 12. Comparison of theoretical mass and energy equation and implementation in Modelica.

	Theoretical equation	Implementation in Modelica
Mass conservation equation of medium (water containing *L. pneumophila* and nutrients)	$V \cdot \frac{d\rho}{dt} = \rho_{in} \cdot v_{in} \cdot A_{in} - \rho_{out} \cdot v_{out} \cdot A_{out}$	*der(m)=mb_flow*
Mass conservation equation of *L. pneumophila* and nutrients	$V \cdot \frac{dC}{dt} = C_{in} \cdot v_{in} \cdot A_{in} - C_{out} \cdot v_{out} \cdot A_{out} + \dot{C}$	*der(mC)=mbC_flow+C_flow_internal*

Energy conservation equation of medium	$\rho \cdot V \cdot \left(\frac{d}{dt}u\right) = \rho \cdot v_{in} \cdot A_{in} \cdot h_{in} + \rho \cdot v_{out} \cdot A_{out} \cdot h_{out} + Q_{cond} + \Phi$	*der(U)=Hb_flow+Q_flow* $\Phi = 0$

In Buildings library, the mass and energy conservation equation can be found in the MixingVolume model. In *Figure A3.1*, the Diagram view of the MixingVolume is shown.

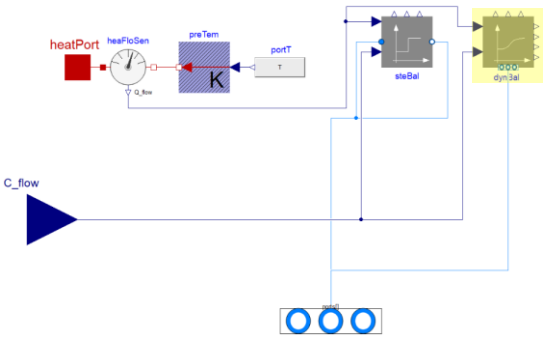


Figure A3.1 Diagram view of MixingVolume model.

In the Text view (*Table 13*), the following code can be found.

Table 13. Implementation of mass and energy conservation equation in Modelica.

Model MixingVolume extends Buildings.Fluid.MixingVolumes.BaseClasses.PartialMixingVolume	**MixingVolume** MixingVolume is an extension of PartialMixingVolume
Model PartialMixingVolume extends Buildings.Fluid.Interfaces.LumpedVolumeDeclarations "contains parameters and medium properties that are used in the lumped volume model" … Buildings.Fluid.Interfaces.ConservationEquation steBal (…) if useSteadyStateTwoPort "Model for dynamic energy conservation" … Buildings.Fluid.Interfaces.ConservationEquation dynBal (final simplify_mWat_flow = simplify_mWat_flow, redeclare final package Medium = Medium, final energyDynamics = energyDynamics, final massDynamics = massDynamics, final p_start = p_start, final T_start = T_start, final X_start = X_start, final C_start = C_start, final C_nominal = C_nominal, final fluidVolume = V, final initialize_p = Initialize_p, m(start=V*rho_start), nPorts=nPorts, final mSenFac=mSenFac) if not useSteadyStateTwoPort "Model for dynamic energy conservation"	**PartialMixingVolume** This is a lumped volume model with the following properties: *p, T, X, C*. It contains the whole mixture volume, in which the number of trace substances is defined (i.e., *L. pneumophila* and nutrients). The lumped volume model contains two ways to solve the conservation Equations (steBal and dynBal). In our models, dynBal, the model to solve the energy conservation dynamically, has been chosen.
Model ConservationEquation "Lumped volume with mass and energy conservation" … Modelica.SIunits.Energy U(start=fluidVolume*rho_start*Medium.specificInternal Energy(Medium.setState_pTX(T=T_start, p=p_start, X=X_start[1:Medium.nXi])) + (T_start - Medium.reference_T)*CSen, nominal = 1E5) "Internal energy of fluid";	**ConservationEquation** The lumped volume works with *T* (temperature), while the conservation equation works with *u* (specificInternalEnergy). *u* is specified in the Medium model. Therefore, a transition to *h* (enthalpy) needs to happen. This is

equation
for i in 1:Medium.nC loop
mbC_flow[i] = sum(ports_mC_flow[:,i]);
end for;
mb_flow = sum(ports.m_flow);
Hb_flow = sum(ports_H_flow);
// Energy and mass conservation equations
if energyDynamics == Modelica.Fluid.Types.Dynamics.SteadyState then
0 = Hb_flow + Q_flow;
else **der(U) = Hb_flow + Q_flow**;
end if;
if massDynamics == Modelica.Fluid.Types.Dynamics.SteadyState then
0 = mb_flow + (if simplify_mWat_flow then 0 else mWat_flow_internal);
else **der(m) = mb_flow** + (if simplify_mWat_flow then 0 else mWat_flow_internal);
end if;
if substanceDynamics == Modelica.Fluid.Types.Dynamics.SteadyState then
zeros(Medium.nXi) = mbXi_flow + mWat_flow_internal * s;
else der(mXi) = mbXi_flow + mWat_flow_internal * s;
end if;
if traceDynamics == Modelica.Fluid.Types.Dynamics.SteadyState then
zeros(Medium.nC) = mbC_flow + C_flow_internal;
else **der(mC) = mbC_flow + C_flow_internal**;
end if;
	added in the package Water of the Building library, by using the function specificInternalEnergy (input *T*).
	
	Energy conservation equation
	
	Mass conservation equation of water
	
	Mass conservation equation of *L. pneumophila* and nutrients. The value for *C_flow_internal* is calculated in our own developed components (part of our own DHW library), thus not belonging to the Buildings library.

redeclare function extends specificInternalEnergy "Return specific internal energy"
extends Modelica.Icons.Function;
algorithm
// u := cv_const*(state.T - T0) - reference_p/d_const;
u := cv_const*(state.T - T0);
end specificInternalEnergy;
	specificInternalEnergy
	This function computes the specific internal energy of the fluid, but neglects the (small) influence of the pressure term *p/d*.

package Water "Package with model for liquid water with constant density" … function enthalpyOfLiquid "Return the specific enthalpy of liquid" extends Modelica.Icons.Function; input Modelica.SIunits.Temperature T "Temperature"; output Modelica.SIunits.SpecificEnthalpy h "Specific enthalpy"; algorithm h := cp_const*(T-reference_T); end enthalpyOfLiquid;	**Water** In package Water, the function enthalpyOfLiquid is specified.

Momentum conservation

While the mass and energy conservation equations are written in the PartialMixingVolume, the momentum conservation equation is written for each flow element (e.g., pipe, boiler, pump) in the code of that specific component. The difference is that the momentum equations take place

between two volume components, i.e., two mixing volumes. So, for a pipe model, the total volume of the pipe is split into a predefined number of segments (an array containing nNodes of MixingVolumes) along the flow path, thus containing nNodes mass and energy conservation equations. Furthermore, only one equation is performed to calculate the pressure drop for the whole (e.g., pipe) model, meaning the transfer of momentum between the fluid and an adjacent surface is modelled using a lumped approach (*Table 14*).

The momentum balance equation as specified in *Annex 3* is *Equation 34*.

$$\rho \cdot V \cdot \frac{d\vec{v}}{dt} = \rho \cdot v_{in}^2 \cdot A_{in} - \rho \cdot v_{out}^2 \cdot A_{in} + \rho \cdot g_x - \frac{dP}{dx} + \nabla(\mu \cdot \nabla v_x) \quad (34)$$

In the Buildings library, a simplification is made by implementing a pressure-based equation based on Bernoulli (*Equation 35*).

$$0 = \frac{{v_2}^2}{2g} - \frac{{v_1}^2}{2g} + (h_2 - h_1) + (\frac{P_2}{\rho g} - \frac{P_1}{\rho g}) + (\Delta h_f + \Delta h_m + \Delta h_p) \quad (35)$$

Table 14. Comparison of theoretical momentum equation and implementation in Modelica.

	Theoretical equation	**Implementation in Modelica**
Momentum conservation	$0 = \frac{{v_2}^2}{2g} - \frac{{v_1}^2}{2g} + (h_2 - h_1) + (\frac{P_2}{\rho g} - \frac{P_1}{\rho g}) + (\Delta h_f + \Delta h_m + \Delta h_p)$	$\Delta p = \rho \cdot g \cdot \Delta h_f$ Assumptions: $v_1 = v_2$: Diameter of pipe is constant $h_1 = h_2$: Horizontal pipe $\Delta h_p = 0$ $\Delta h_m = \Delta h_f$: Minor losses (e.g., fittings)

An example of the implementation of the momentum conservation in a pipe component is given in *Table 15*. The principle of the used pipe model "Pipe_2_Leg", is similar to the Pipe model in Buildings library, except that it contains extra equations to calculate the *L. pneumophila* concentration in water and biofilm.

Table 15. Implementation of momentum conservation equation in Modelica.

```
Model Pipe_2_Leg "Pipe with finite volume discretization along flow path"
  Extends DHW.LegionellaModels.Pipe_1_Leg(
    diameter=sqrt(4*m_flow_nominal/rho_default/v_nominal/
    Modelica.Constants.pi),
    dp_nominal=2*dpStraightPipe_nominal,
    preDro(dp(nominal=length*10)),
    redeclare replaceable package Medium = DHW.LegionellaModels.WaterLeg,
    vol(use_C_flow=true));
…
final parameter Modelica.SIunits.PressureDifference dpStraightPipe_nominal(displayU
nit="Pa")=Modelica.Fluid.Pipes.BaseClasses.WallFriction.Detailed.pressureLoss_m_fl
ow(
    m_flow=m_flow_nominal,
    rho_a=rho_default,
    rho_b=rho_default,
    mu_a=mu_default,
    mu_b=mu_default,
    length=length,
    diameter=diameter,
    roughness=roughness,
    m_flow_small=m_flow_small)
    "Pressure loss of a straight pipe at m_flow_nominal";
```

Pipe_2_Leg
Pipe model with roughness is an extension of a pipe model without roughness (Pipe_1_Leg). A pressure drop is given to Pipe_1_Leg, that is calculated as dpStraightPipe_nominal. This pressure drop, taking into account the pressure losses of a straight pipe, is multiplied by two to incorporate the minor losses Δh_m.

The total pressure drop, dp_nominal, is calculated in Pipe_2_Leg with the function pressureLoss_m_flow based on the material roughness.

In case the velocity is not the nominal velocity, this pressure drop is adapted by the model preDro, which is available in Pipe_1_Leg.

```
model Pipe_1_Leg "Model of a pipe with finite volume discretization along the
  flow path"
 extends Modelica.Icons.Example;
 extends Buildings.Fluid.Interfaces.LumpedVolumeDeclarations;
 extends Buildings.Fluid.Interfaces.PartialTwoPortInterface(final show_T=true);
 extends Buildings.Fluid.Interfaces.TwoPortFlowResistanceParameters(final
```

Pipe_1_Leg
LumpedVolumeDeclarations is a record that contains the parameters and medium properties that are used in the lumped volume model. TwoPortFlowResistanceParameters is a record

computeFlowResistance=(abs(dp_nominal) > Modelica.Constants.eps)); Buildings.Fluid.FixedResistances.PressureDrop preDro(…); Buildings.Fluid.MixingVolumes.MixingVolume [nSeg] vol(…)	that contains parameters that are used to compute the pressure drop in models that have one fluid stream. Furthermore the pipe model contains an array of MixingVolumes and a model that calculates the pressure drop. preDro to relate dp_nominal to m, in case m is not m_nominal. MixingVolume to calculate mass and energy conservation equations.
Function pressureLoss_m_flow Re := diameter*abs(m_flow)/(crossArea*mu); lambda2 := if Re <= Re1 then 64*Re else (if Re >= Re2 then 0.25*(Re/Math.log10(Delta/3.7 + 5.74/Re^0.9))^2 Else interpolateInRegion2(Re, Re1, Re2, Delta)); dp :=length*mu*mu/(2*rho*diameter*diameter*diameter)* (if m_flow >= 0 then lambda2 else -lambda2);	**pressureLoss_m_flow** To calculate the pressure drop associated with frictional effects (Δh_f),the Darcy-Weisbach equation is applied, stating that $\Delta p = \zeta \cdot \frac{L}{D} \cdot \frac{\rho \cdot v^2}{2}$. The pressure drop due to wall friction is computed as product of dynamic pressure and a loss factor ζ. The loss factor $\zeta$is based on the Colebrook-White equation, this equation is translated in Modelica in the function pressureLoss_m_flow. A problem arises because the Colebrook-White equation is an iterative formula. To solve this, an explicit variation of the Colebrook-White equation is used, namely the Swamee-Jain equation, for flow in a completely filled pipe with circular section.

Annex 6 - *Understanding the simulation log basics*

When you run a simulation in Dymola, a simulation log is generated. The statistics listed in *Table 16* can be considered the key performance indicators of the simulation computational performance.

Table 16. Key performance indicators of the simulation computational performance (Claytex 2016)

Simulation log variable	General definition of variable
CPU-time for integration	The total CPU-time of the simulation.
CPU-time for one GRID interval	The CPU-time to calculate one grid interval.
Number of result points	The total number of simulation steps stored by Dymola in the result file
Number of GRID points	Evenly spaced points with spacing determined from “Interval length” or “number of intervals” and the simulation time.
Number of (successful) steps	Total number of simulation steps calculated by the solver. The result points are extrapolated from these steps.
Number of F-evaluations	Number of times equations used to calculate the gradient of the states were run.
Number of H-evaluations	Number of times the crossing functions had to be calculated. These functions are used to determine when an event occurs.
Number of Jacobian-evaluations	The Jacobian is utilised by the solver method during the solving process. The solver method requests that the Jacobian be updated throughout the simulation.
Number of (model) time events	Events that are generated at a given time.
Number of (U) time events	Events that are generated when discrete input signal changes occur.
Number of state events	

Minimum integration stepsize	A real elementary relation changes its value, for example “x>2” changes its value.
Maximum integration stepsize	Minimum stepsize used during simulation.
Maximum integration order	Maximum stepsize used during simulation. The maximum integration order used by the solver.